OAK RIDGE National Laboratory

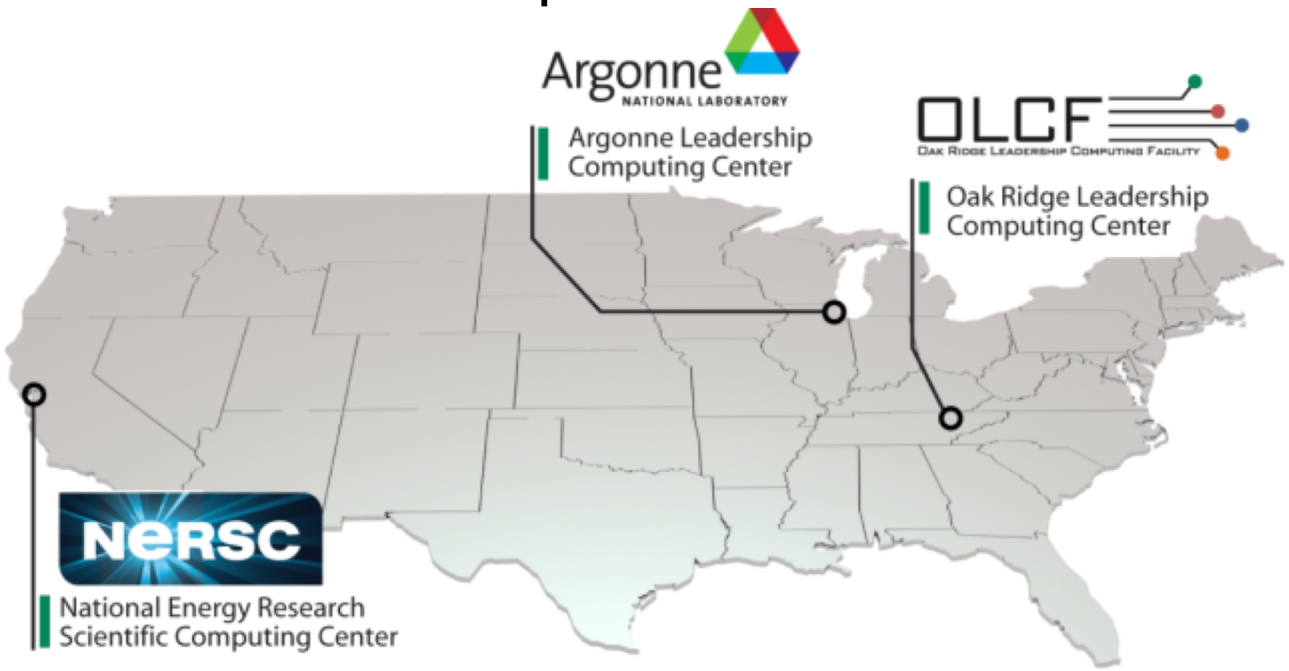
GPU Accelerated Computing on Summit

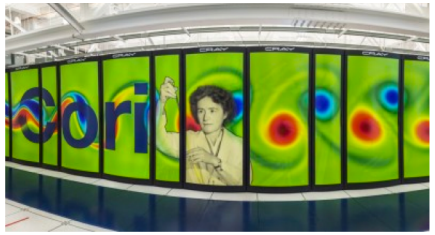
Tom Papatheodore & Graham Lopez
Oak Ridge Leadership Computing Facility (OLCF)

SIAM Conference on Computational Science and Engineering (CSE19)
Spokane, WA
27 Feb 2019

U.S. DEPARTMENT OF ENERGY

DOE's Office of Science Computation User Facilities





NERSC
Cori is 30 PF

ALCF
Theta is 12 PF

OLCF
Summit is 200 PF

- DOE is leader in open High-Performance Computing
- Provide the world's most powerful computational tools for open science
- Access is free to researchers who publish
- Boost US competitiveness
- Attract the best and brightest researchers

What is a Leadership Computing Facility (LCF)?

- Collaborative DOE Office of Science user-facility program at ORNL and ANL
- Mission: Provide the computational and data resources required to solve the most challenging problems.
- 2-centers/2-architectures to address diverse and growing computational needs of the scientific community

- Highly competitive user allocation programs (INCITE, ALCC).
- Projects receive 10x to 100x more resource than at other generally available centers.
- LCF centers partner with users to enable science & engineering breakthroughs (Liaisons, Catalysts).

OAK RIDGE National Laboratory

Argonne NATIONAL LABORATORY

ORNL has systematically delivered a series of leadership-class systems

On scope • On budget • Within schedule

18.5 TF
2004
Cray X1E
Phoenix

25 TF
2005
Cray XT3
Jaguar

54 TF
2006
Cray XT3
Jaguar

62 TF
2007
Cray XT4
Jaguar

263 TF
2008
Cray XT4
Jaguar

1 PF
2008
Cray XT5
Jaguar

2.5 PF
2009
Cray XT5
Jaguar

1000-fold improvement in 8 years

27 PF
2012
Cray XK7
Titan

Titan, six years old in October 2018, continues to deliver world-class science research in support of our user community. We will operate Titan through 2019 when it will be decommissioned.

OAK RIDGE National Laboratory

We are building on this record of success to enable exascale in 2021

2012
Cray XK7
Titan

2018
IBM
Summit

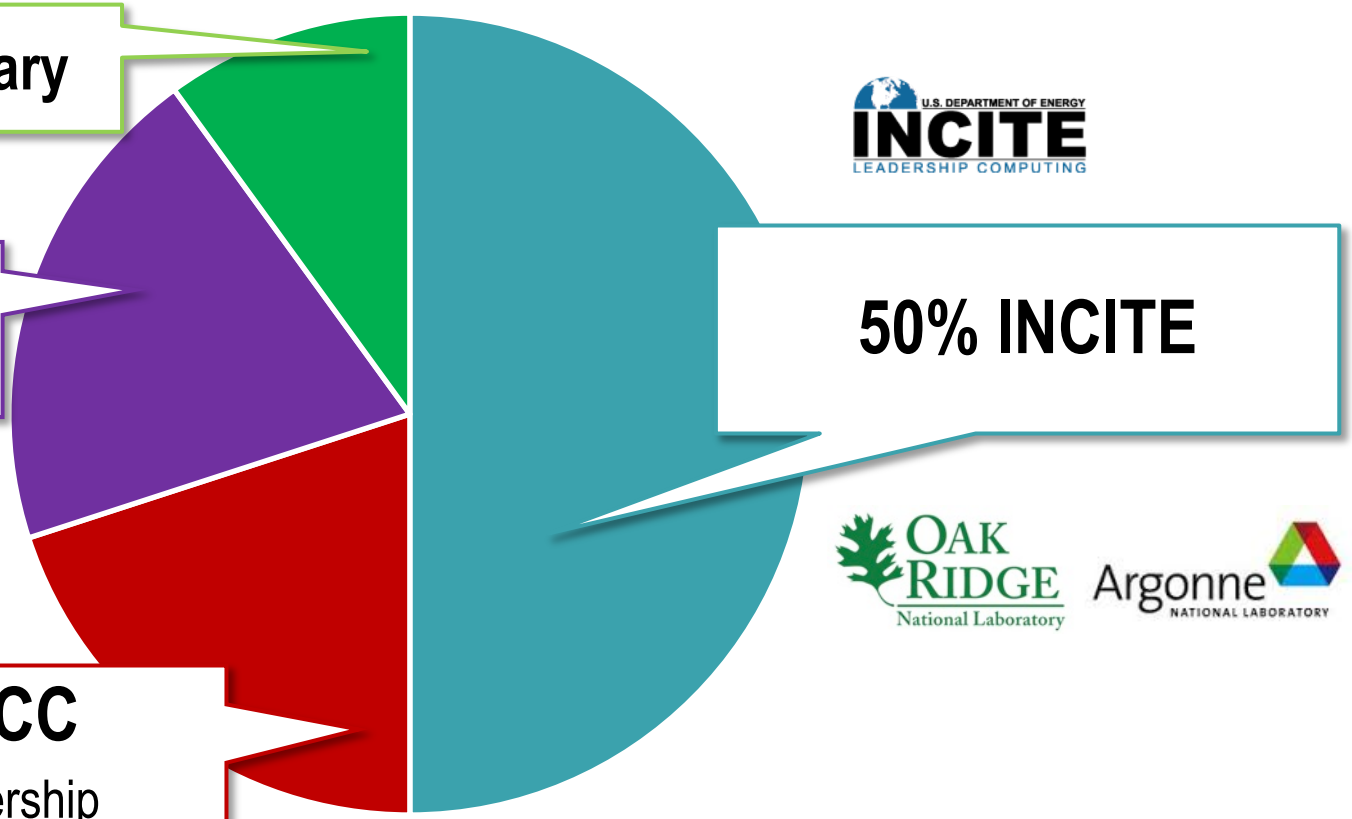
2021
Frontier

Four primary user programs for access to LCF

Distribution of allocable hours

INCITE (Open Science)
- Large allocations (50-250 Mch)
- Solve most challenging problems in science and engineering
- Single simulations use 20%> of system
- Annual call for proposals

10% **Director's Discretionary**



20% ECP
Exascale Computing Project

50% INCITE

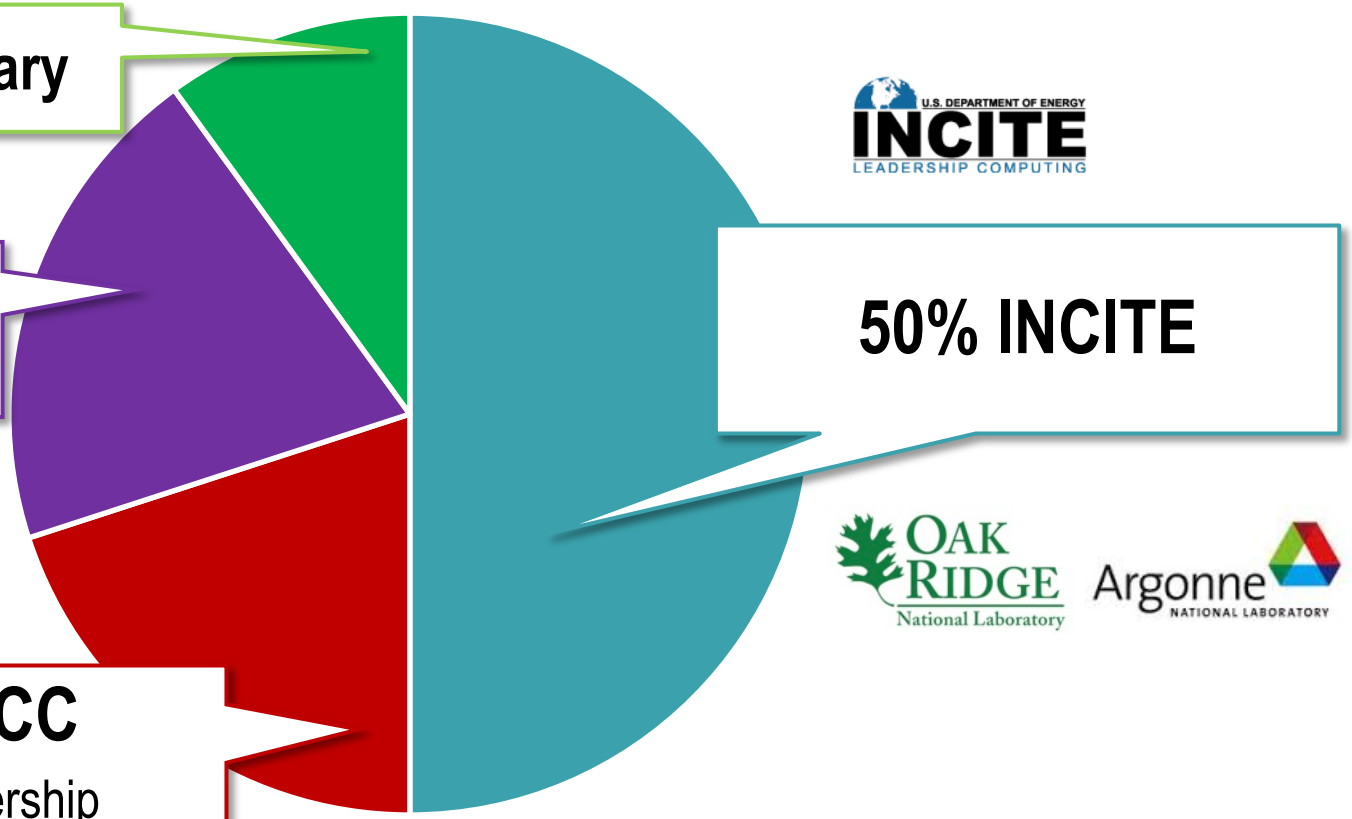
20% ALCC
ASCR Leadership Computing Challenge

Four primary user programs for access to LCF

Distribution of allocable hours

ALCC (DOE Mission Science)
- Large allocations (50-250 Mch)
- Projects inline with mission of DOE
- Annual call for proposals

10% **Director's Discretionary**



20% ECP
Exascale Computing Project

20% ALCC
ASCR Leadership Computing Challenge

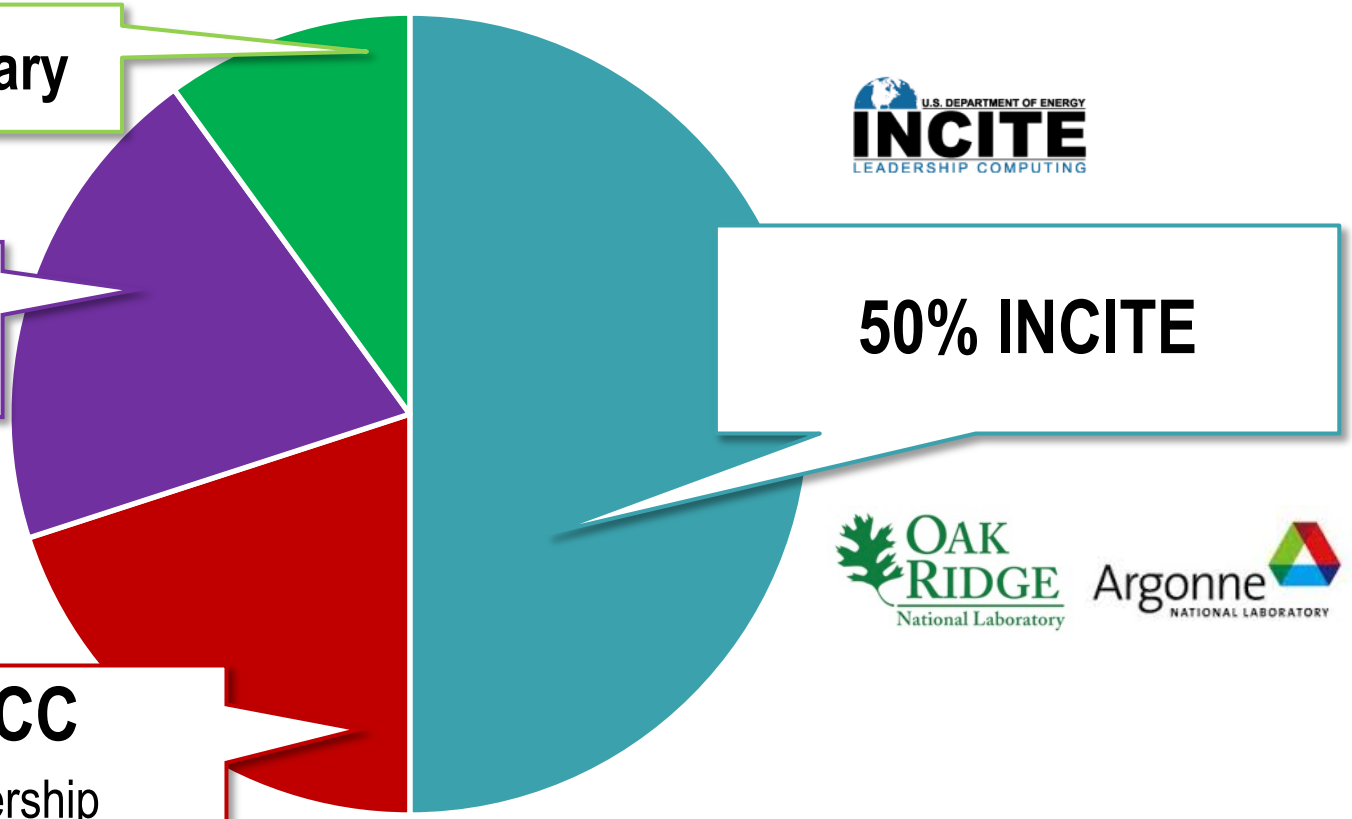
50% INCITE

Four primary user programs for access to LCF

Distribution of allocable hours

ECP
- Projects that are inline with the ECP priorities
- These applications are already chosen

10% **Director's Discretionary**



20% ECP
Exascale Computing Project

50% INCITE

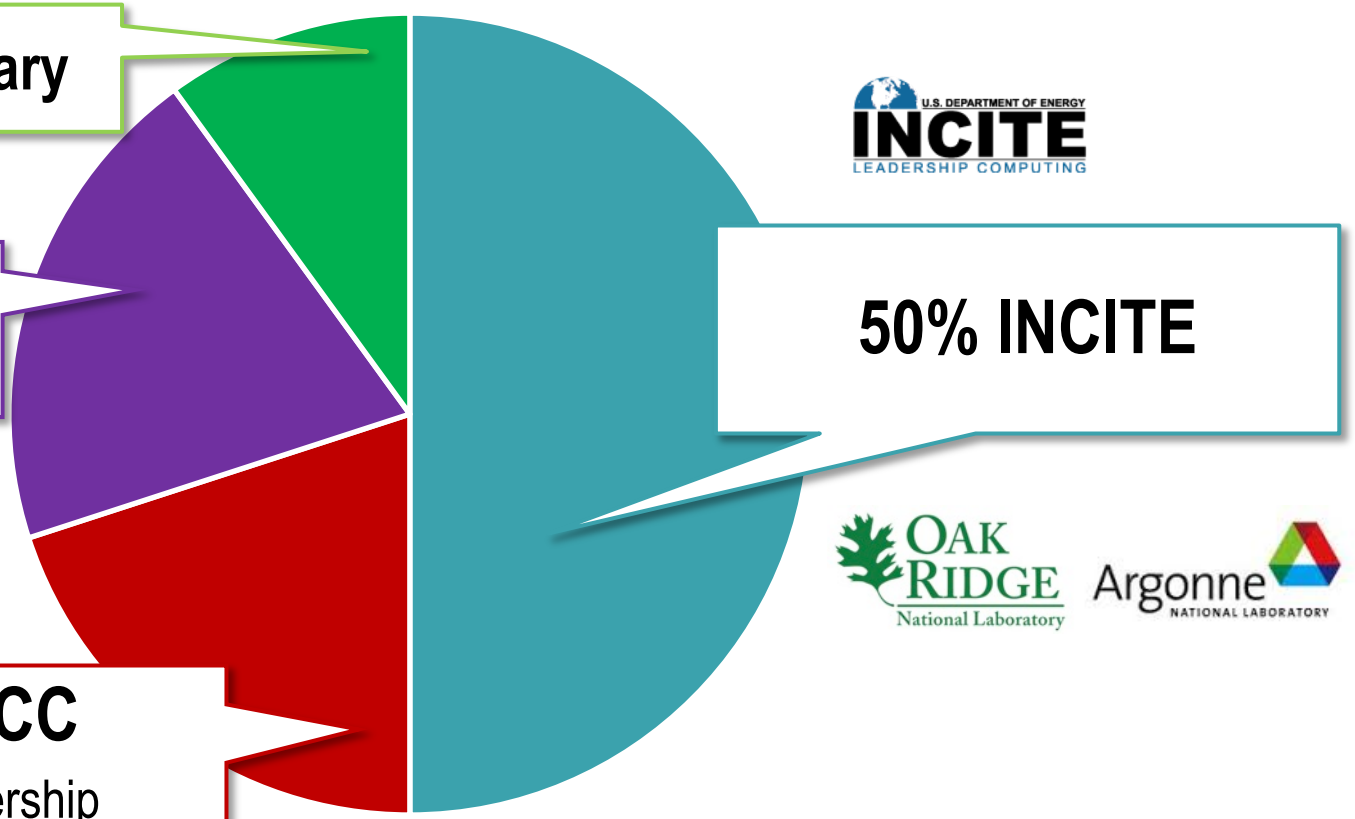
20% ALCC
ASCR Leadership Computing Challenge

Four primary user programs for access to LCF

Distribution of allocable hours

DD
- Smaller allocations (<5 Mch)
- Intended as onramp for new projects
- Preparation for larger allocation programs
- Proposals accepted year round (starting Dec. for Summit)

10% **Director's Discretionary**



20% ECP
Exascale Computing Project

20% ALCC
ASCR Leadership Computing Challenge

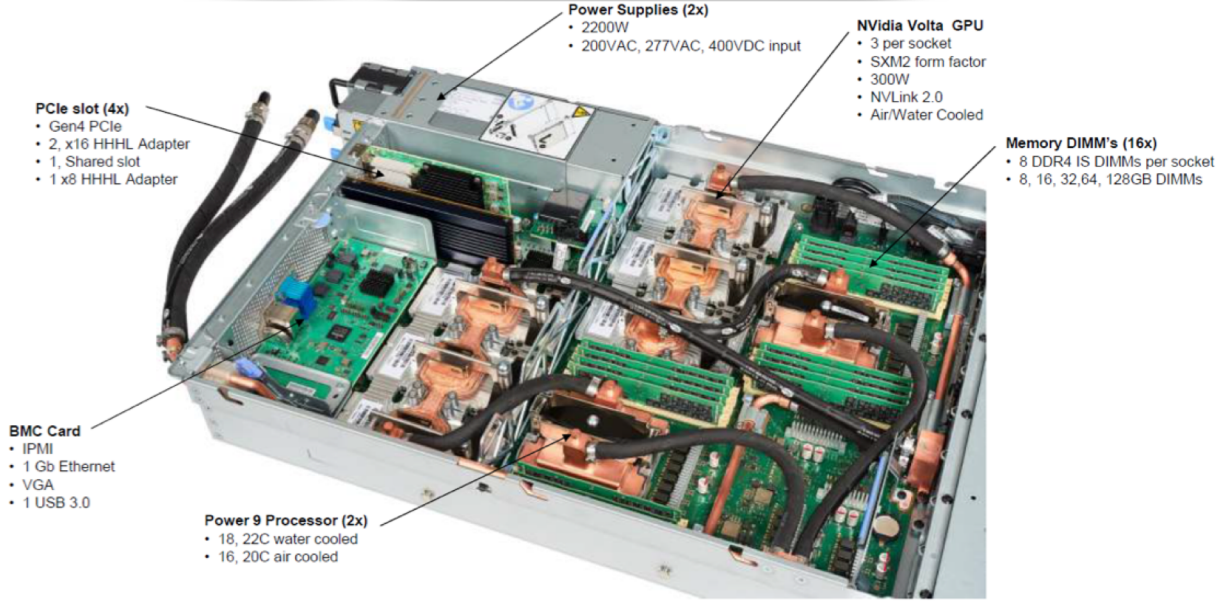
50% INCITE

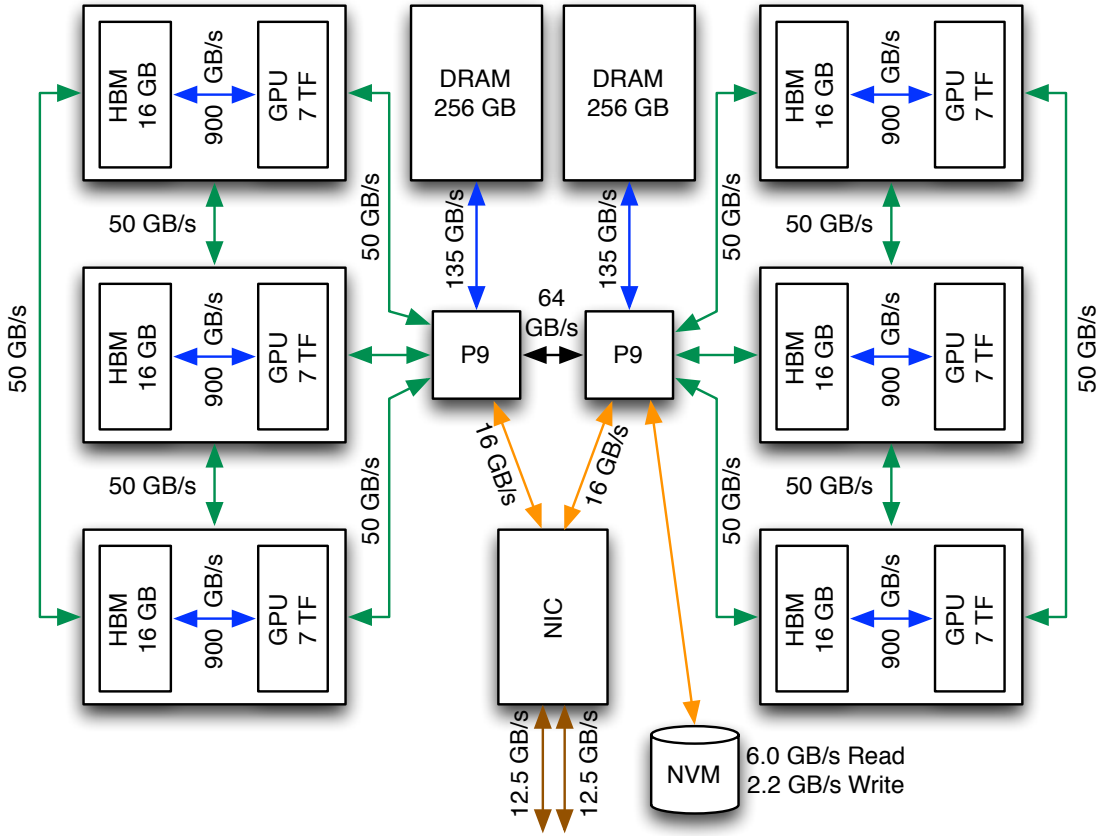
Apply for New OLCF Allocations

Please visit the following page on the OLCF website to learn more about each user program, or to apply:

https://www.olcf.ornl.gov/for-users/getting-started/#request-a-new-allocation

summit





TF	42 TF (6x7 TF)
HBM	96 GB (6x16 GB)
DRAM	512 GB (2x16x16 GB)
NET	25 GB/s (2x12.5 GB/s)
MMsg/s	83

HBM/DRAM Bus (aggregate B/W)
NVLINK
X-Bus (SMP)
PCIe Gen4
EDR IB

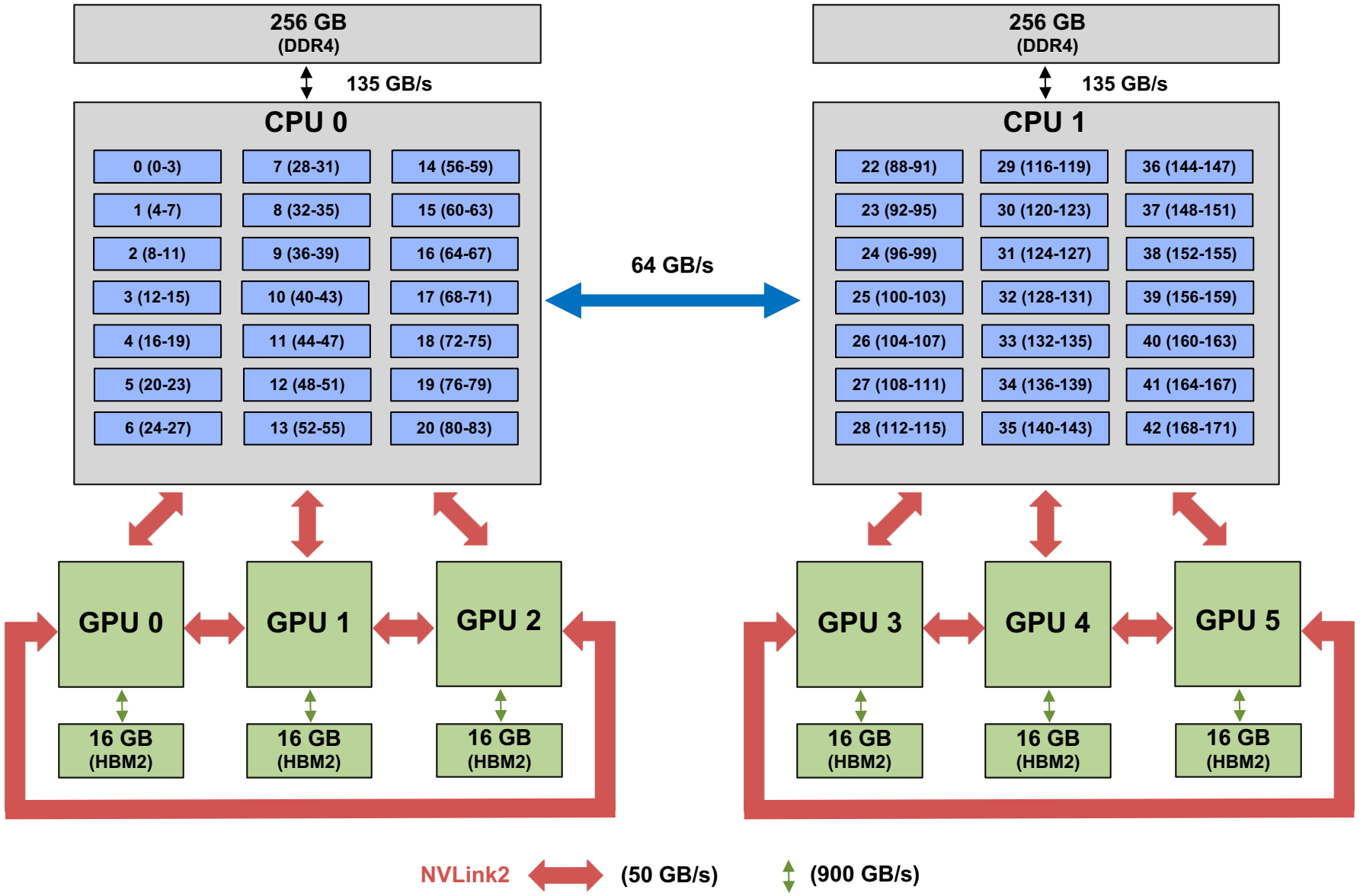
HBM & DRAM speeds are aggregate (Read+Write).
All other speeds (X-Bus, NVLink, PCIe, IB) are bi-directional.

Node Overview

OAK RIDGE National Laboratory

Summit Node

(2) IBM Power9 + (6) NVIDIA Volta V100



OAK RIDGE National Laboratory

Hands-On Session

Outline of Hands-On Session

- Logging Into Ascent and Setting Up Environment
- Heterogeneous (CPU+GPU) Programming Basics
- A Simple Example: Vector Addition
- Jacobi Iteration
  - Serial
  - Single GPU
  - Single GPU (explicit data movement)
  - Multiple GPU (OpenMP + OpenACC)

OAK RIDGE National Laboratory

Logging Into Ascent and Setting Up Environment

Log Into Ascent and Change Directory

1. From the command line:

   `$ ssh USERNAME@login1.ascent.olcf.ornl.gov`

   (This will drop you into the directory `/ccsopen/home/USERNAME`)

2. Change to the following directory:

   `$ cd /gpfs/wolf/gen117/scratch/USERNAME`

Clone Repository and Set up Programming Environment

3. Once in `/gpfs/wolf/gen117/scratch/USERNAME`, clone git repository:

```
$ git clone https://github.com/tom-papatheodore/2019_SIAM_CSE.git
```

4. cd into directory:

```
$ cd 2019_SIAM_CSE
```

5. Run script to set up environment for the tutorial:

```
$ source environment.sh
```

At this point, you prompt should look like this:

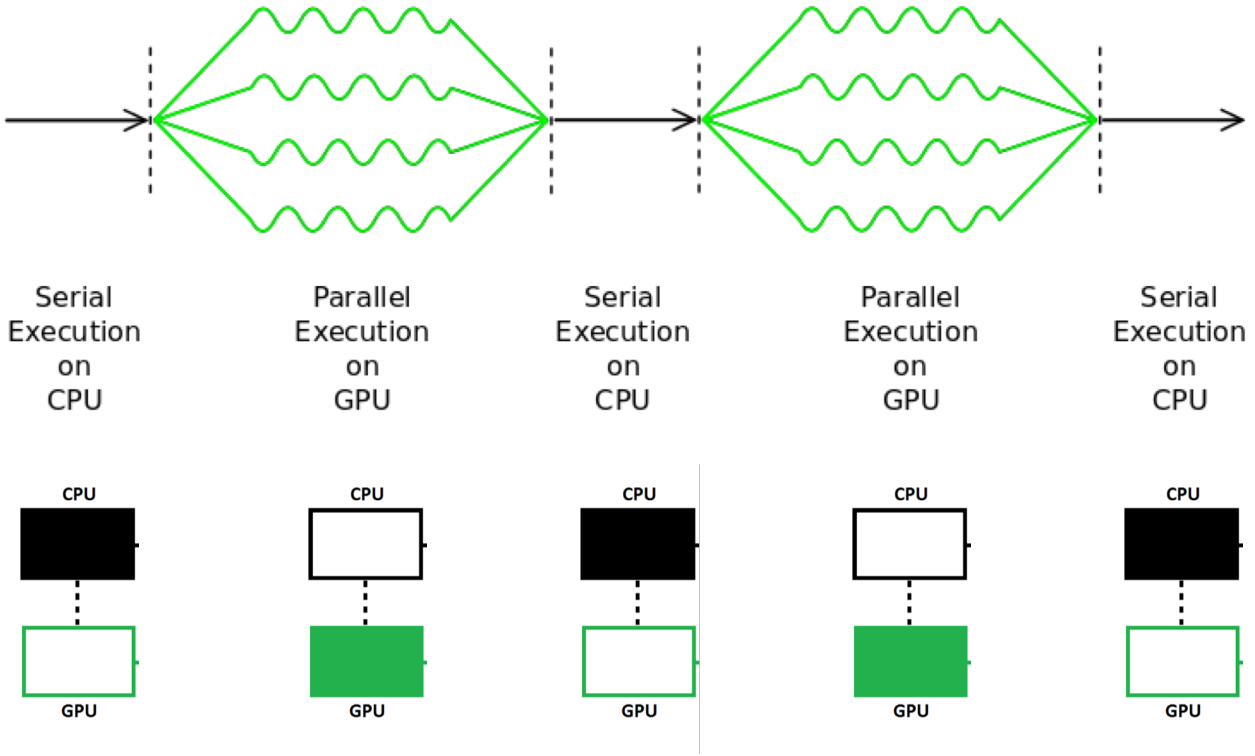
```
[USERNAME@login1: /gpfs/wolf/gen117/scratch/USERNAME/2019_SIAM_CSE]$
```

OAK RIDGE National Laboratory

Heterogeneous Programming Model

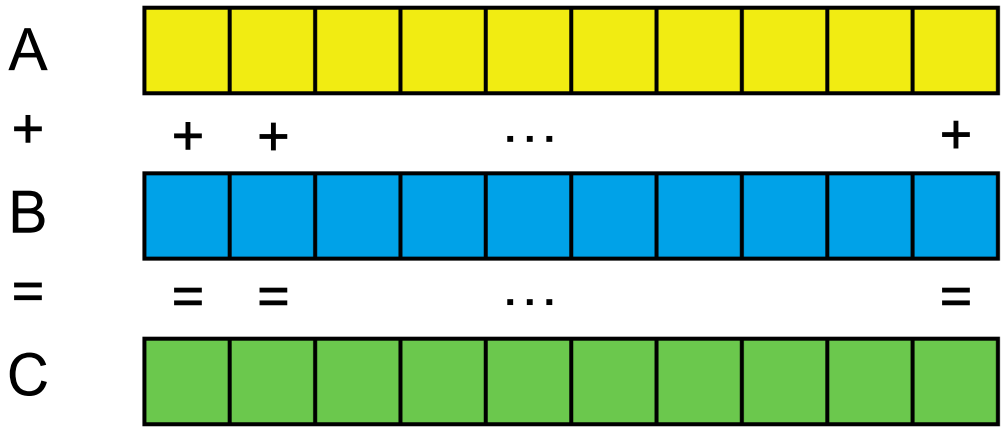
Heterogeneous Programming Model

- Program separated into serial regions (run on CPU) and parallel regions (run on GPU)



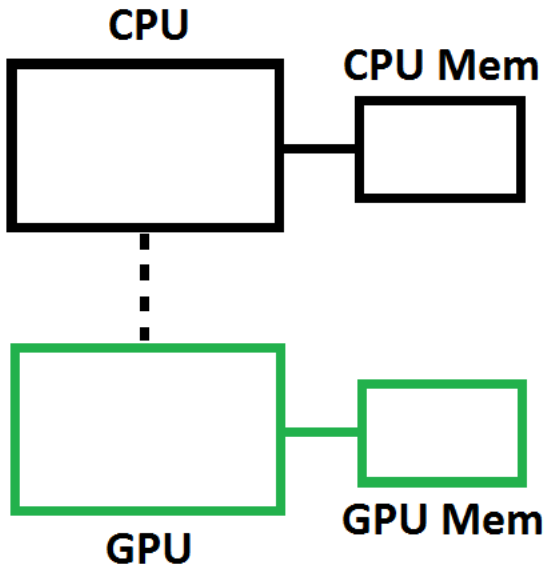
Heterogeneous Programming Model

- Parallel regions consist of many calculations that can be executed independently
  - Data Parallelism (e.g. vector addition)



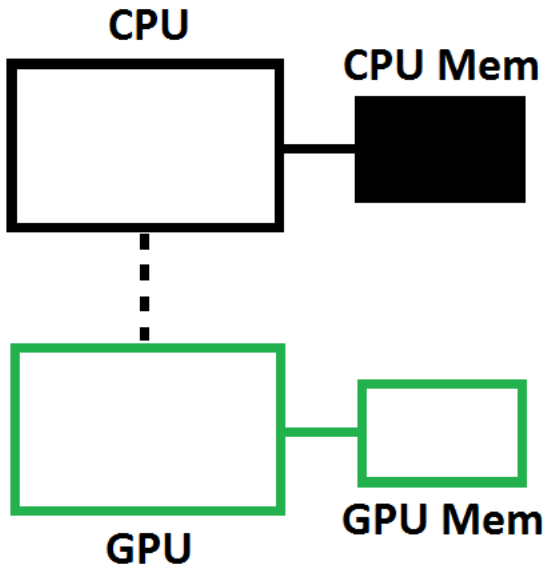
A Basic GPU Program Outline

```
int main(){
  // Allocate memory for array on host
  // Allocate memory for array on device
  // Fill array on host
  // Copy data from host array to device array
  // Do something on device (e.g. vector addition)
  // Copy data from device array to host array
  // Check data for correctness
  // Free Host Memory
  // Free Device Memory
}
```



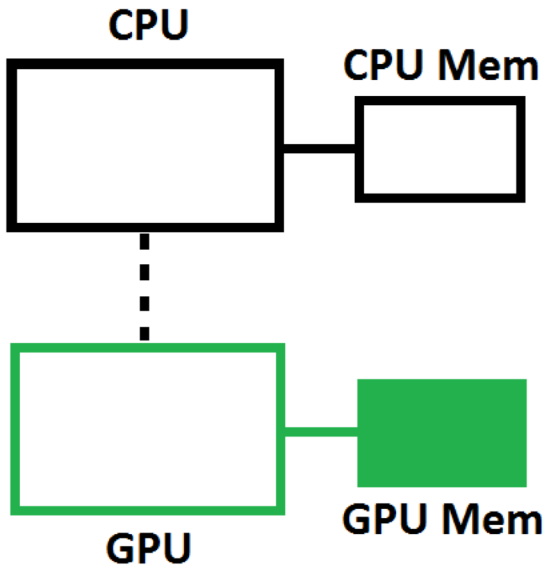
A Basic GPU Program Outline

```
int main(){
  // Allocate memory for array on host
  // Allocate memory for array on device
  // Fill array on host
  // Copy data from host array to device array
  // Do something on device (e.g. vector addition)
  // Copy data from device array to host array
  // Check data for correctness
  // Free Host Memory
  // Free Device Memory
}
```



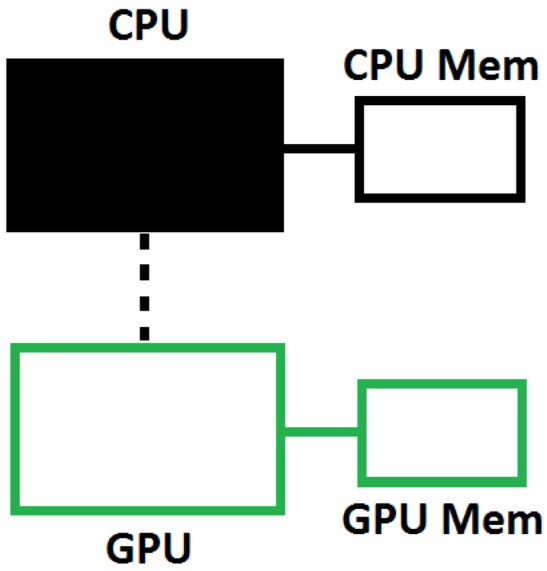
A Basic GPU Program Outline

```
int main(){
  // Allocate memory for array on host
  // Allocate memory for array on device
  // Fill array on host
  // Copy data from host array to device array
  // Do something on device (e.g. vector addition)
  // Copy data from device array to host array
  // Check data for correctness
  // Free Host Memory
  // Free Device Memory
}
```



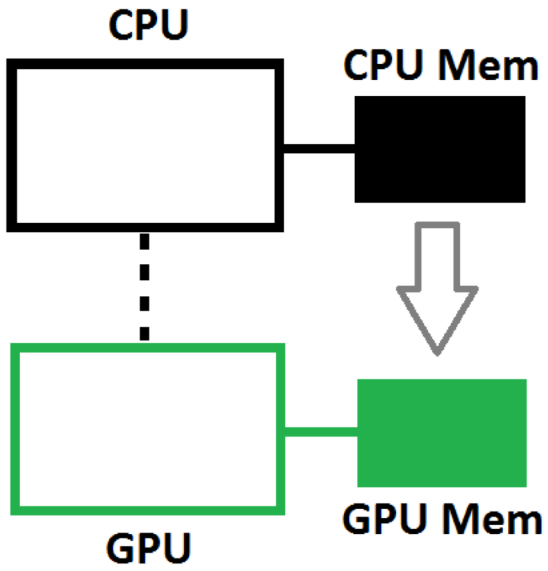
A Basic GPU Program Outline

```
int main(){
  // Allocate memory for array on host
  // Allocate memory for array on device
  // Fill array on host
  // Copy data from host array to device array
  // Do something on device (e.g. vector addition)
  // Copy data from device array to host array
  // Check data for correctness
  // Free Host Memory
  // Free Device Memory
}
```



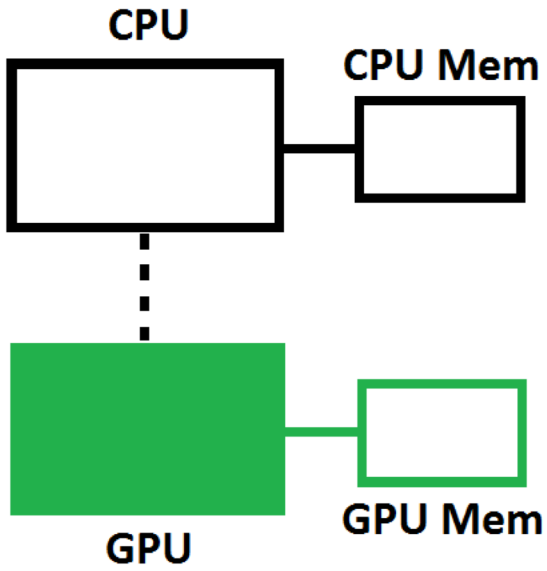
A Basic GPU Program Outline

```
int main(){
  // Allocate memory for array on host
  // Allocate memory for array on device
  // Fill array on host
  // Copy data from host array to device array
  // Do something on device (e.g. vector addition)
  // Copy data from device array to host array
  // Check data for correctness
  // Free Host Memory
  // Free Device Memory
}
```



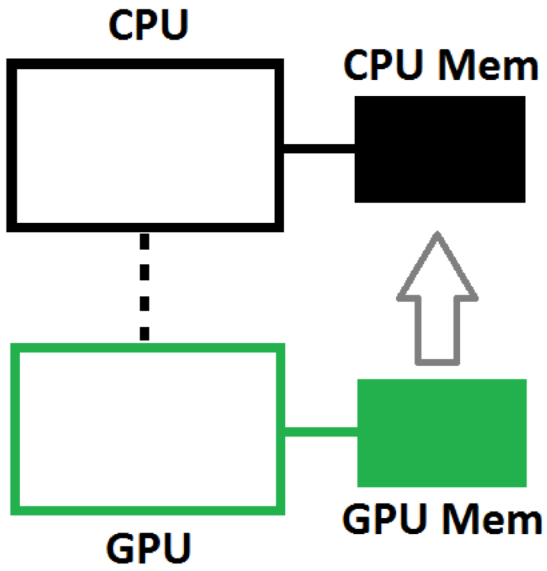
A Basic GPU Program Outline

```
int main(){
  // Allocate memory for array on host
  // Allocate memory for array on device
  // Fill array on host
  // Copy data from host array to device array
  // Do something on device (e.g. vector addition)
  // Copy data from device array to host array
  // Check data for correctness
  // Free Host Memory
  // Free Device Memory
}
```



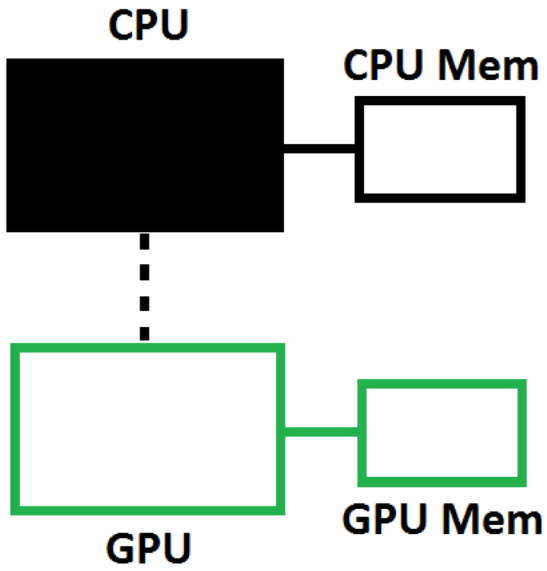
A Basic GPU Program Outline

```
int main(){
  // Allocate memory for array on host
  // Allocate memory for array on device
  // Fill array on host
  // Copy data from host array to device array
  // Do something on device (e.g. vector addition)
  // Copy data from device array to host array
  // Check data for correctness
  // Free Host Memory
  // Free Device Memory
}
```



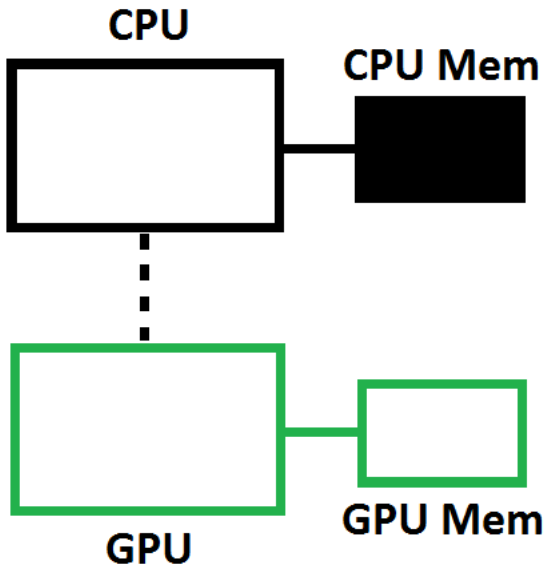
A Basic GPU Program Outline

```
int main(){
  // Allocate memory for array on host
  // Allocate memory for array on device
  // Fill array on host
  // Copy data from host array to device array
  // Do something on device (e.g. vector addition)
  // Copy data from device array to host array
  // Check data for correctness
  // Free Host Memory
  // Free Device Memory
}
```



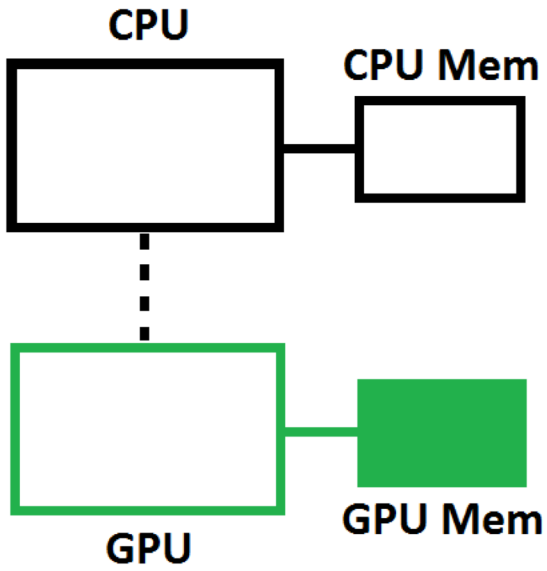
A Basic GPU Program Outline

```
int main(){
  // Allocate memory for array on host
  // Allocate memory for array on device
  // Fill array on host
  // Copy data from host array to device array
  // Do something on device (e.g. vector addition)
  // Copy data from device array to host array
  // Check data for correctness
  // Free Host Memory
  // Free Device Memory
}
```



A Basic GPU Program Outline

```
int main(){
  // Allocate memory for array on host
  // Allocate memory for array on device
  // Fill array on host
  // Copy data from host array to device array
  // Do something on device (e.g. vector addition)
  // Copy data from device array to host array
  // Check data for correctness
  // Free Host Memory
  // Free Device Memory
}
```



OAK RIDGE National Laboratory

A Simple Example: Vector Addition

CUDA Vector Addition

```
#include <stdio.h>
#define N 1048576

__global__ void add_vectors(int *a, int *b, int *c){
    int id = blockDim.x * blockIdx.x + threadIdx.x;
    if(id < N) c[id] = a[id] + b[id];
}

int main(){
    size_t bytes = N*sizeof(int);

    int *A = (int*)malloc(bytes);
    int *B = (int*)malloc(bytes);
    int *C = (int*)malloc(bytes);

    int *d_A, *d_B, *d_C;
    cudaMalloc(&d_A, bytes);
    cudaMalloc(&d_B, bytes);
    cudaMalloc(&d_C, bytes);

    for(int i=0; i<N; i++){
        A[i] = 1;
        B[i] = 2;
    }

    cudaMemcpy(d_A, A, bytes, cudaMemcpyHostToDevice);
    cudaMemcpy(d_B, B, bytes, cudaMemcpyHostToDevice);

    int thr_per_blk = 256;
    int blk_in_grid = ceil( float(N) / thr_per_blk );
    add_vectors<<< blk_in_grid, thr_per_blk >>>(d_A, d_B, d_C);

    cudaMemcpy(C, d_C, bytes, cudaMemcpyDeviceToHost);

    free(A);
    free(B);
    free(C);
    cudaFree(d_A);
    cudaFree(d_B);
    cudaFree(d_C);

    return 0;
}
```

CUDA Vector Addition

```
#include <stdio.h>
#define N 1048576

__global__ void add_vectors(int *a, int *b, int *c){
    int id = blockDim.x * blockIdx.x + threadIdx.x;
    if(id < N) c[id] = a[id] + b[id];
}

int main(){
    size_t bytes = N*sizeof(int);

    int *A = (int*)malloc(bytes);
    int *B = (int*)malloc(bytes);
    int *C = (int*)malloc(bytes);

    int *d_A, *d_B, *d_C;
    cudaMalloc(&d_A, bytes);
    cudaMalloc(&d_B, bytes);
    cudaMalloc(&d_C, bytes);

    for(int i=0; i<N; i++){
        A[i] = 1;
        B[i] = 2;
    }

    cudaMemcpy(d_A, A, bytes, cudaMemcpyHostToDevice);
    cudaMemcpy(d_B, B, bytes, cudaMemcpyHostToDevice);

    int thr_per_blk = 256;
    int blk_in_grid = ceil( float(N) / thr_per_blk );
    add_vectors<<< blk_in_grid, thr_per_blk >>>(d_A, d_B, d_C);

    cudaMemcpy(C, d_C, bytes, cudaMemcpyDeviceToHost);

    free(A);
    free(B);
    free(C);
    cudaFree(d_A);
    cudaFree(d_B);
    cudaFree(d_C);

    return 0;
}
```

OpenACC Vector Addition

```
#include <stdio.h>
#include <stdlib.h>
#define N 1048576

int main(){
    size_t bytes = N*sizeof(int);

    int *A = (int*)malloc(bytes);
    int *B = (int*)malloc(bytes);
    int *C = (int*)malloc(bytes);

    for(int i=0; i<N; i++){
        A[i] = 1;
        B[i] = 2;
    }

    #pragma acc parallel loop
    for(int i=0; i<N; i++){
        C[i] = A[i] + B[i];
    }

    free(A);
    free(B);
    free(C);

    return 0;
}
```

OAK RIDGE National Laboratory

Jacobi Iteration

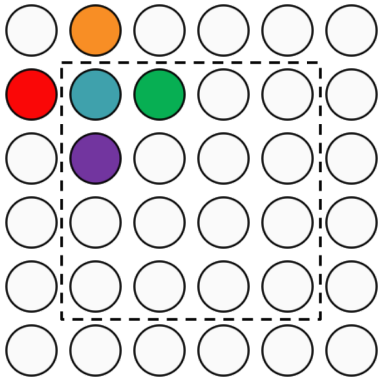
Jacobi Iteration – Problem Description

Use Jacobi Iteration to solve 2D Poisson equation with periodic boundary conditions:

$$\Delta A(y,x) = e^{-10(x*x + y*y)}$$

Execute a Jacobi Step on the Inner Points

$$A_{k+1}(iy,ix) = rhs(iy,ix) - (A_k(iy,ix-1) + A_k(iy,ix+i) + A_k(iy-1,ix) + A_k(iy+1,ix))$$



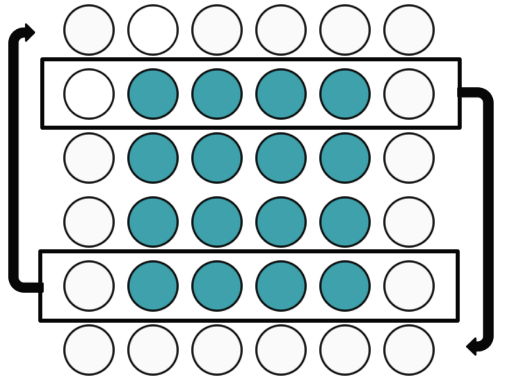
```
for (int iy = 1; iy < NY-1; iy++)
{
    for( int ix = 1; ix < NX-1; ix++ )
    {
        Anew[iy][ix] = -0.25 * (rhs[iy][ix] - ( A[iy][ix+1] + A[iy][ix-1]
                                              + A[iy-1][ix] + A[iy+1][ix] ));
        error = fmax( error, fabs(Anew[iy][ix]-A[iy][ix]));
    }
}
```

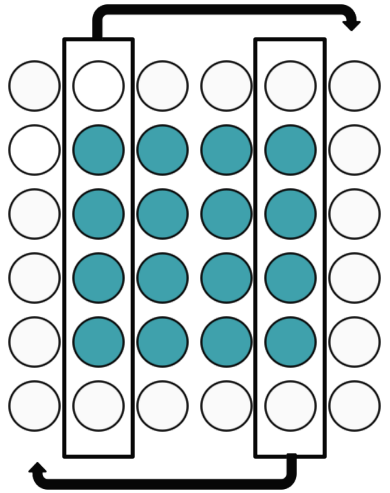
Copy Values of Anew to A

```
for (int iy = 1; iy < NY-1; iy++)
{
    for( int ix = 1; ix < NX-1; ix++ )
    {
        A[iy][ix] = Anew[iy][ix];
    }
}
```

Apply Periodic Boundary Conditions

```
//Periodic boundary conditions
for( int ix = 1; ix < NX-1; ix++ )
{
        A[0][ix]      = A[(NY-2)][ix];
        A[(NY-1)][ix] = A[1][ix];
}
for (int iy = 1; iy < NY-1; iy++)
{
        A[iy][0]      = A[iy][(NX-2)];
        A[iy][(NX-1)] = A[iy][1];
}
```





Serial Version

`2019_SIAM_CSE/jacobi/1_serial`

Serial Runtime

Compile the code

```
$ make
pgcc -Minfo -fast -c poisson2d.c
main:
     54, Generated vector simd code for the loop
         FMA (fused multiply-add) instruction(s) generated
     65, Memory zero idiom, loop replaced by call to __c_mzero8
     84, FMA (fused multiply-add) instruction(s) generated
     90, Generated vector simd code for the loop containing reductions
    100, Memory copy idiom, loop replaced by call to __c_mcopy8
    107, Loop not fused: dependence chain to sibling loop
         Generated vector simd code for the loop
         Residual loop unrolled 2 times (completely unrolled)
    112, Loop not fused: function call before adjacent loop
         Loop unrolled 8 times
pgcc -Minfo -fast poisson2d.o -o run
```

Run the code (on single CPU core)

```
$ bsub submit.lsf
Job <11536> is submitted to default queue <batch>.


$ jobstat
--------------- Running Jobs: 1 (1 of 16 nodes, 6.25%) ---------------
JobId  Username  Project  Nodes  Remain  StartTime       JobName
11536  t4p       GEN117   1      8:48    02/24 10:03:14  serial
--------------- Eligible Jobs: 0 -------------------------------------
--------------- Blocked Jobs: 0 --------------------------------------


$ less output.11536
Jacobi relaxation Calculation: 4096 x 4096 mesh
    0, 0.250000
  100, 0.249940
  200, 0.249880
  300, 0.249821
  400, 0.249761
  500, 0.249702
  600, 0.249642
  700, 0.249583
  800, 0.249524
  900, 0.249464
Elapsed Time (s):

...
...
```

(Enter q to quit/exit less)

2019_SIAM_CSE/jacobi/1_serial

Single GPU Version

`2019_SIAM_CSE/jacobi/2_single_gpu`

Difference From Serial Version

- Added OpenACC pragmas to inform compiler where to offload work to GPU

```
#pragma acc kernels
```

- Added (optional) serial version to compare with timing and results of GPU version

```
// Set to 1 to run serial test, otherwise 0
int serial_test = 0;
```

Runtime of Single GPU Version

Compile the code

```
$ make
pgcc -acc -Minfo=acc -ta=tesla:cc70 -fast -c poisson2d.c
main:
    117, Generating implicit copyin(A[:][:],rhs[1:4094][1:4094])
         Generating implicit copyout(Anew[1:4094][1:4094])
    118, Loop is parallelizable
    120, Loop is parallelizable
         Accelerator kernel generated
         Generating Tesla code
        118, #pragma acc loop gang, vector(4) /* blockIdx.y threadIdx.y */
        120, #pragma acc loop gang, vector(32) /* blockIdx.x threadIdx.x */
        124, Generating implicit reduction(max:error)
    128, Generating implicit copyin(Anew[1:4094][1:4094])
         Generating implicit copyout(A[1:4094][1:4094])
    129, Loop is parallelizable
    131, Loop is parallelizable
         Accelerator kernel generated
         Generating Tesla code
        129, #pragma acc loop gang, vector(4) /* blockIdx.y threadIdx.y */
        131, #pragma acc loop gang, vector(32) /* blockIdx.x threadIdx.x */
    138, Generating implicit copy(A[:][1:4094])
    139, Loop is parallelizable
         Accelerator kernel generated
         Generating Tesla code
        139, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
    144, Generating implicit copy(A[1:4094][:])
    145, Loop is parallelizable
         Accelerator kernel generated
         Generating Tesla code
        145, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
pgcc -acc -Minfo=acc -ta=tesla:cc70 -fast poisson2d.o -o run
```

Run the code (on single GPU)

```
$ bsub submit.lsf

$ less output
Jacobi relaxation Calculation: 4096 x 4096 mesh
Parallel Execution...
    0, 0.250000
  100, 0.249940
  200, 0.249880
  300, 0.249821
  400, 0.249761
  500, 0.249702
  600, 0.249642
  700, 0.249583
  800, 0.249524
  900, 0.249464
Elapsed Time (s) - Parallel:
```

2019_SIAM_CSE/jacobi/2_single_gpu

Runtime of Single GPU Version

Compile the code

```
$ make
pgcc -acc -Minfo=acc -ta=tesla:cc70 -fast -c poisson2d.c
main:
    117, Generating implicit copyin(A[:][:],rhs[1:4094][1:4094])
         Generating implicit copyout(Anew[1:4094][1:4094])
    118, Loop is parallelizable
    120, Loop is parallelizable
         Accelerator kernel generated
         Generating Tesla code
        118, #pragma acc loop gang, vector(4) /* blockIdx.y threadIdx.y */
        120, #pragma acc loop gang, vector(32) /* blockIdx.x threadIdx.x */
        124, Generating implicit reduction(max:error)
    128, Generating implicit copyin(Anew[1:4094][1:4094])
         Generating implicit copyout(A[1:4094][1:4094])
    129, Loop is parallelizable
    131, Loop is parallelizable
         Accelerator kernel generated
         Generating Tesla code
        129, #pragma acc loop gang, vector(4) /* blockIdx.y threadIdx.y */
        131, #pragma acc loop gang, vector(32) /* blockIdx.x threadIdx.x */
    138, Generating implicit copy(A[:][1:4094])
    139, Loop is parallelizable
         Accelerator kernel generated
         Generating Tesla code
        139, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
    144, Generating implicit copy(A[1:4094][:])
    145, Loop is parallelizable
         Accelerator kernel generated
         Generating Tesla code
        145, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
pgcc -acc -Minfo=acc -ta=tesla:cc70 -fast poisson2d.o -o run
```

Run the code (on single GPU)

```
$ bsub submit.lsf

$ less output
Jacobi relaxation Calculation: 4096 x 4096 mesh
Parallel Execution...
    0, 0.250000
  100, 0.249940
  200, 0.249880
  300, 0.249821
  400, 0.249761
  500, 0.249702
  600, 0.249642
  700, 0.249583
  800, 0.249524
  900, 0.249464
Elapsed Time (s) - Parallel: 127.2326
```

Why are we slower than serial version??

How can we answer such questions?

2019_SIAM_CSE/jacobi/2_single_gpu

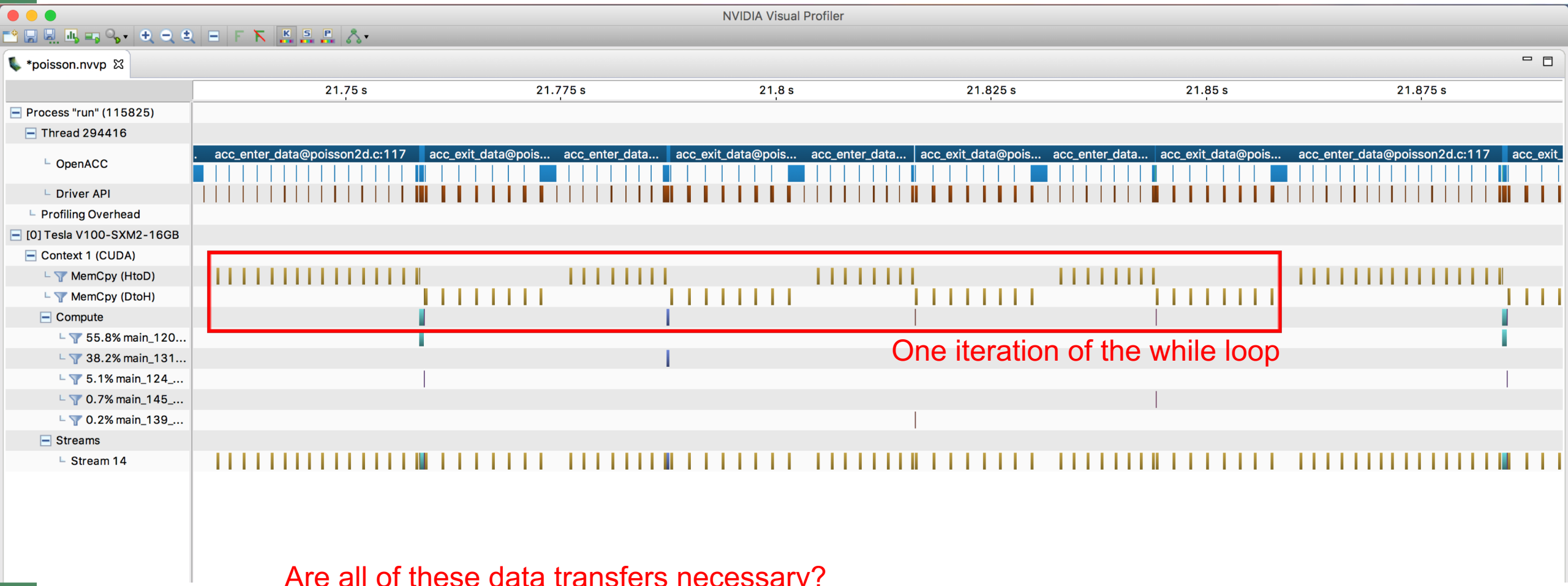
Using NVIDIA's NVProf Profiler, we see…

```
$ bsub submit.lsf   (jsrun --smpiargs="none" -n1 -c1 -g1 -a1 nvprof ./run)

$ less output
==56446== NVPROF is profiling process 56446, command: ./run
==56446== Profiling application: ./run

Jacobi relaxation Calculation: 4096 x 4096 mesh
Parallel Execution...
    0, 0.250000
  100, 0.249940
  200, 0.249880
  300, 0.249821
  400, 0.249761
  500, 0.249702
  600, 0.249642
  700, 0.249583
  800, 0.249524
  900, 0.249464
Elapsed Time (s) - Parallel: 130.9012

==56446== Profiling result:
            Type  Time(%)      Time     Calls       Avg       Min       Max  Name
 GPU activities:   53.55%  14.4180s     41000  351.66us  1.3110us  382.72us  [CUDA memcpy HtoD]
                   42.84%  11.5335s     33000  349.50us  1.7590us  362.53us  [CUDA memcpy DtoH]
                    2.01%  541.55ms      1000  541.55us  539.61us  546.01us  main_120_gpu
                    1.38%  372.18ms      1000  372.18us  369.47us  376.64us  main_131_gpu
                    0.19%  49.816ms      1000  49.815us  48.448us  51.231us  main_124_gpu__red
                    0.02%  6.1174ms      1000  6.1170us  5.7270us  6.9760us  main_145_gpu
                    0.01%  2.1649ms      1000  2.1640us  1.8880us  2.8480us  main_139_gpu
```

Do we really need all these data transfers?

Let's look at visual output (and compiler output) to see what's going on…

Using NVIDIA's Visual Profiler, we see…



Are all of these data transfers necessary?

Let's look back at the code to see how data should be transferred…

Where are arrays actually needed?

```
// Main iteration loop
while ( error > tol && iter < iter_max )
{
    error = 0.0;

    #pragma acc kernels
    for (int iy = 1; iy < NY-1; iy++)
    {
        for( int ix = 1; ix < NX-1; ix++ )
        {
            Anew[iy][ix] = -0.25 * (rhs[iy][ix] - ( A[iy][ix+1] + A[iy][ix-1]
                                                  + A[iy-1][ix] + A[iy+1][ix] ));
            error = fmax( error, fabs(Anew[iy][ix]-A[iy][ix]));
        }
    }

    #pragma acc kernels
    for (int iy = 1; iy < NY-1; iy++)
    {
        for( int ix = 1; ix < NX-1; ix++ )
        {
            A[iy][ix] = Anew[iy][ix];
        }
    }

    //Periodic boundary conditions
    #pragma acc kernels
    for( int ix = 1; ix < NX-1; ix++ )
    {
            A[0][ix]      = A[(NY-2)][ix];
            A[(NY-1)][ix] = A[1][ix];
    }
    #pragma acc kernels
    for (int iy = 1; iy < NY-1; iy++)
    {
            A[iy][0]      = A[iy][(NX-2)];
            A[iy][(NX-1)] = A[iy][1];
    }

    if((iter % 100) == 0) printf("%5d, %0.6f\n", iter, error);

    iter++;
}
```

- `Anew` is updated
- `A` and `rhs` are not updated
- Reduction performed on `error`

- `A` is updated
- `Anew` is not updated

But nowhere is this while loop are `Anew`, `A`, or `rhs` needed on the CPU!

- `A` is updated

- `A` is updated

Single GPU Version with Data Regions

`2019_SIAM_CSE/jacobi/3_single_gpu_data`

Difference From Initial GPU Version

- Added a data region around while loop

```
#pragma acc data ...
{
  while loop
}
```

- Still have (optional) serial version to compare with timing and results of GPU version

```
// Set to 1 to run serial test, otherwise 0
int serial_test = 0;
```

Runtime of Single GPU Version with Data Directives

Compile the code

```
$ make
pgcc -acc -Minfo=acc -ta=tesla:cc70 -fast -c poisson2d.c
main:
    112, Generating copyin(rhs[:][:])
         Generating create(Anew[:][:])
         Generating copy(A[:][:])
    121, Loop is parallelizable
    123, Loop is parallelizable
         Accelerator kernel generated
         Generating Tesla code
        121, #pragma acc loop gang, vector(4) /* blockIdx.y threadIdx.y */
        123, #pragma acc loop gang, vector(32) /* blockIdx.x threadIdx.x */
        127, Generating implicit reduction(max:error)
    132, Loop is parallelizable
    134, Loop is parallelizable
         Accelerator kernel generated
         Generating Tesla code
        132, #pragma acc loop gang, vector(4) /* blockIdx.y threadIdx.y */
        134, #pragma acc loop gang, vector(32) /* blockIdx.x threadIdx.x */
    142, Loop is parallelizable
         Accelerator kernel generated
         Generating Tesla code
        142, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
    148, Loop is parallelizable
         Accelerator kernel generated
         Generating Tesla code
        148, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
pgcc -acc -Minfo=acc -ta=tesla:cc70 -fast poisson2d.o -o run
```

Run the code (on single GPU)

```
$ bsub submit.lsf

$ less output
Jacobi relaxation Calculation: 4096 x 4096 mesh
Parallel Execution...
    0, 0.250000
  100, 0.249940
  200, 0.249880
  300, 0.249821
  400, 0.249761
  500, 0.249702
  600, 0.249642
  700, 0.249583
  800, 0.249524
  900, 0.249464
Elapsed Time (s) - Parallel:
```

2019_SIAM_CSE/jacobi/3_single_gpu_data

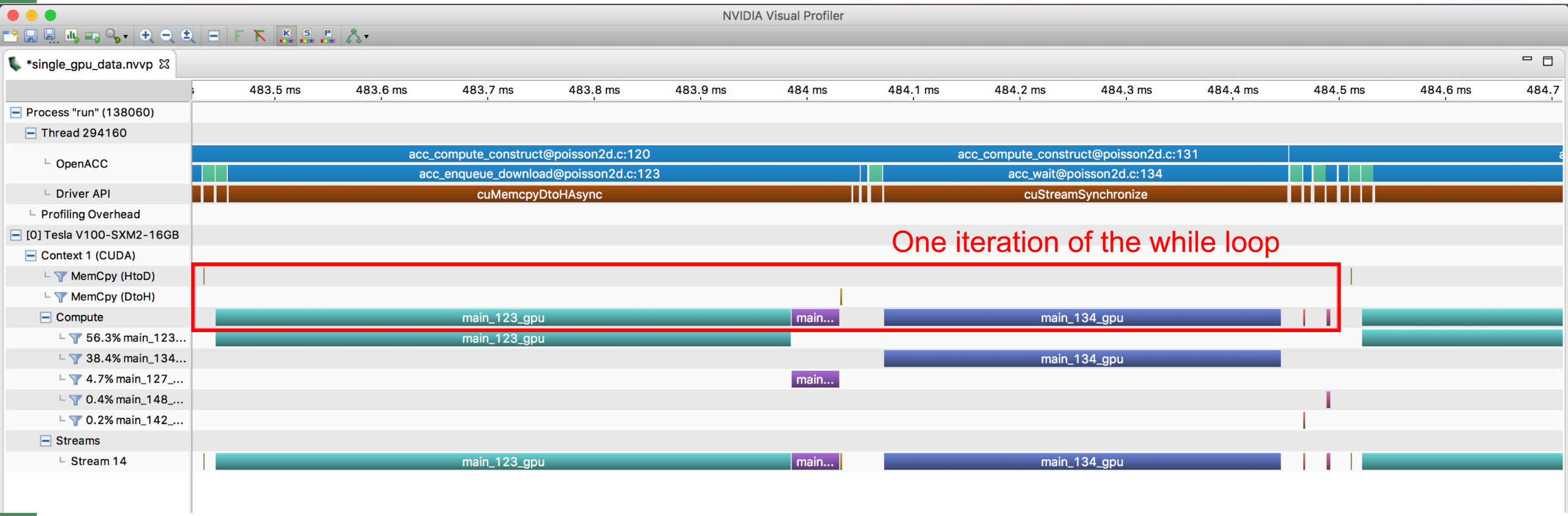
Using NVIDIA's NVProf Profiler, we see…

```
$ bsub submit.lsf   (jsrun --smpiargs="none" -n1 -c1 -g1 -a1 nvprof ./run)

$ less output
==139388== NVPROF is profiling process 139388, command: ./run
==139388== Profiling application: ./run

Jacobi relaxation Calculation: 4096 x 4096 mesh
Parallel Execution...
    0, 0.250000
  100, 0.249940
  200, 0.249880
  300, 0.249821
  400, 0.249761
  500, 0.249702
  600, 0.249642
  700, 0.249583
  800, 0.249524
  900, 0.249464
Elapsed Time (s) - Parallel:   1.9883

==139388== Profiling result:
            Type  Time(%)      Time     Calls       Avg       Min       Max  Name
 GPU activities:   55.51%  539.46ms      1000  539.46us  537.53us  542.75us  main_123_gpu
                   38.02%  369.46ms      1000  369.46us  366.65us  373.57us  main_134_gpu
                    4.76%  46.220ms      1000  46.219us  43.935us  51.040us  main_127_gpu__red
                    0.72%  7.0198ms      1016  6.9090us  1.2160us  360.06us  [CUDA memcpy HtoD]
                    0.47%  4.5286ms      1009  4.4880us  1.5990us  359.04us  [CUDA memcpy DtoH]
                    0.35%  3.4053ms      1000  3.4050us  3.0400us  4.4480us  main_148_gpu
                    0.18%  1.7651ms      1000  1.7650us  1.6320us  2.2080us  main_142_gpu
```

~60X faster with explicit data management

Data transfers are no longer dominating run time.

Using NVIDIA's Visual Profiler, we see…



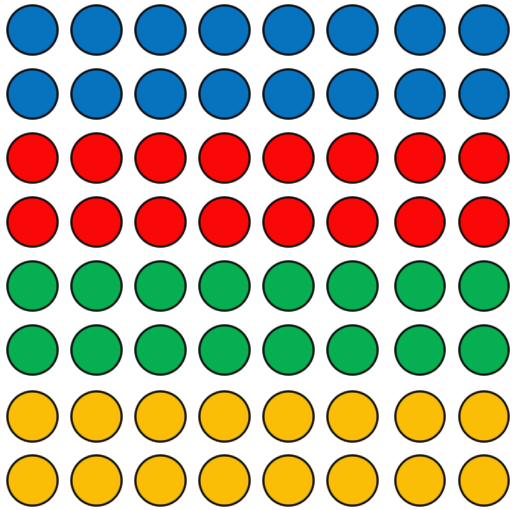
We have eliminated the unnecessary data transfers.

Multiple GPU Version (OpenMP + OpenACC)

`2019_SIAM_CSE/jacobi/4_multiple_gpu_openmp`

Differences from Single GPU Version

- Each OpenMP thread calculates its own loop bounds for its portion of the domain and uses its own GPU.



OpenMP Thread 0 ⇒ GPU 0

OpenMP Thread 1 ⇒ GPU 1

OpenMP Thread 2 ⇒ GPU 2

OpenMP Thread 3 ⇒ GPU 3

Differences from Single GPU Version

```
#pragma omp parallel default(shared) firstprivate(num_threads, thread_num){}
```

```
#ifdef _OPENMP
    num_threads = omp_get_num_threads();
    thread_num  = omp_get_thread_num();
#endif /* _OPENMP */


#ifdef _OPENACC
    int num_devices = acc_get_num_devices(acc_device_nvidia);
    int device_num  = thread_num % num_devices;
    acc_set_device_num(device_num, acc_device_nvidia);
#endif /* _OPENACC */
```

Map OpenMP threads to available GPUs

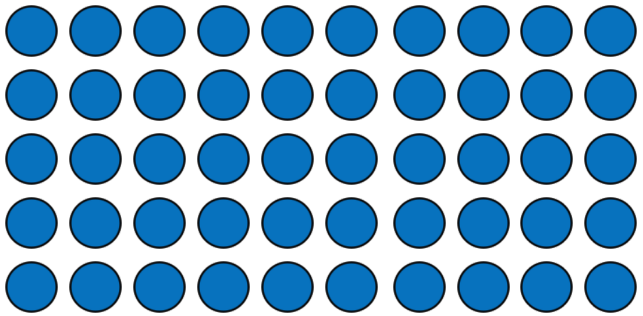
```
#pragma omp master
{
// Set rhs
for (int iy = 1; iy < NY-1; iy++)
{
    for(int ix = 1; ix < NX-1; ix++ )
    {
        const double x = -1.0 + (2.0*ix/(NX-1));
        const double y = -1.0 + (2.0*iy/(NY-1));
        rhs[iy][ix] = exp(-10.0*(x*x + y*y));
    }
}
} /* pragma omp master */
```

Only the master thread needs to set value of rhs

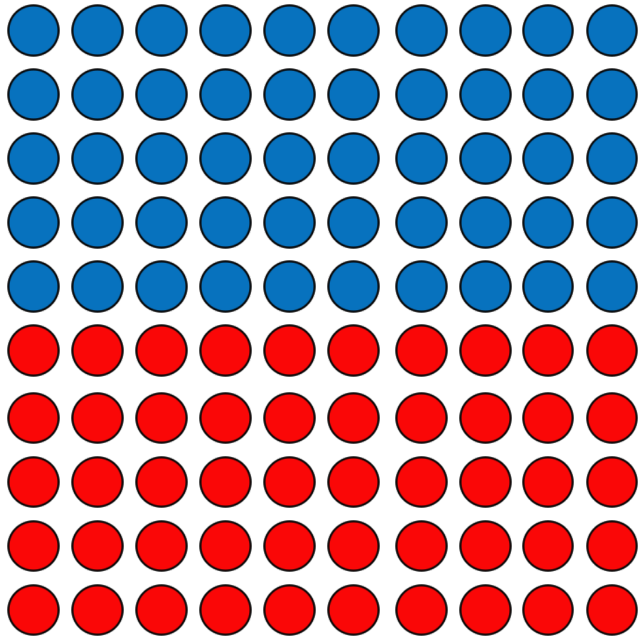
Differences from Single GPU Version

```
#pragma acc data copy(A[(iy_start-1):(iy_end-iy_start)+2][0:NX]) \
                 copyin(rhs[iy_start:(iy_end-iy_start)][0:NX]) \
                 create(Anew[iy_start:(iy_end-iy_start)][0:NX])
```

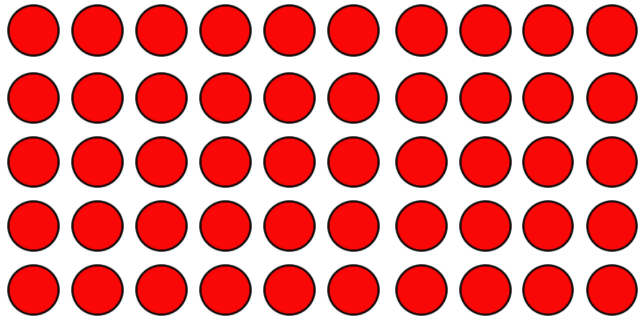
Thread 0's copy of its rows of A (on GPU 0)



CPU copy of A



Thread 1's copy of its rows of A (on GPU 1)

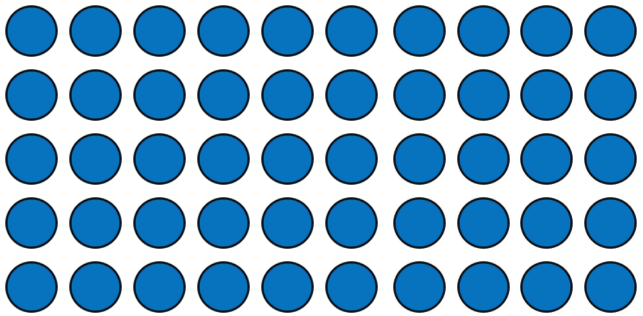


Differences from Single GPU Version

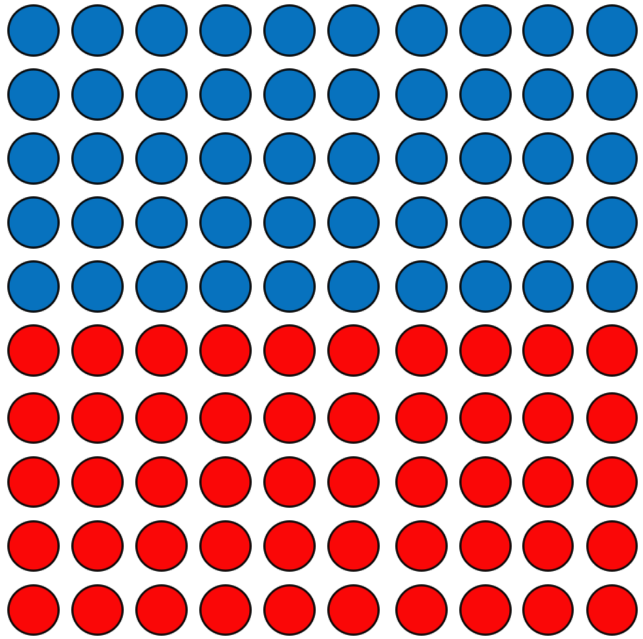
```
#pragma acc kernels
for (int iy = iy_start; iy < iy_end; iy++)
{
    for( int ix = ix_start; ix < ix_end; ix++ )
    {
        Anew[iy][ix] = -0.25 * (rhs[iy][ix] - ( A[iy][ix+1] + A[iy][ix-1]
                                              + A[iy-1][ix] + A[iy+1][ix] ));
        error = fmax( error, fabs(Anew[iy][ix]-A[iy][ix]));
    }
}
```

After GPUs update their values of A, the CPU copy is no longer correct

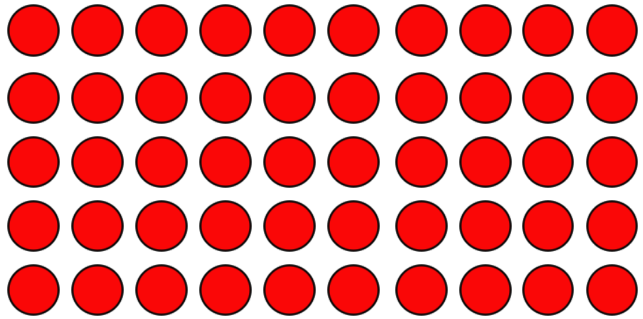
Thread 0's copy of its rows of A (on GPU 0)



CPU copy of A



Thread 1's copy of its rows of A (on GPU 1)

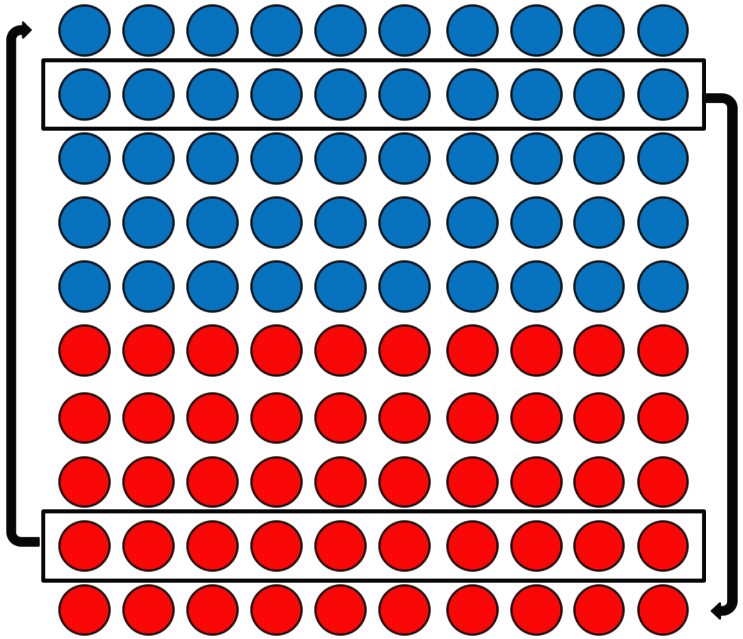


Differences from Single GPU Version

Recall that boundary conditions must be updated for A matrix as a whole

- But each GPU only has its rows of A
- So some data must be passed back to CPU

CPU copy of A

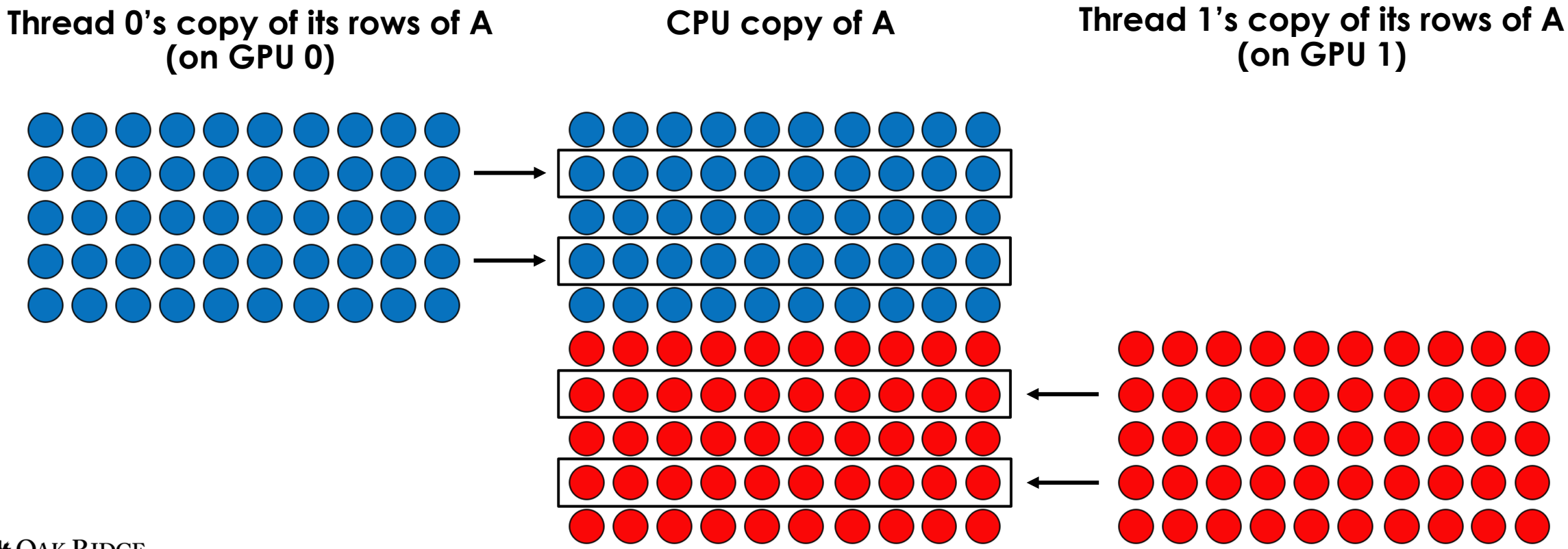


2019_SIAM_CSE/jacobi/4_multiple_gpu_openmp

Differences from Single GPU Version

```
#pragma acc update self(A[iy_start:1][0:NX], A[(iy_end-1):1][0:NX])
```

Each thread updates the "shared" CPU copy of A with its "2nd-to-top" row and "2nd-to-bottom" row



Differences from Single GPU Version

Top/Bottom Boundaries

```
if(0 == (iy_start-1))
{
    for( int ix = 1; ix < NX-1; ix++ )
    {
        A[0][ix]      = A[(NY-2)][ix];
    }
}
```

```
if((NY-1) == (iy_end))
{
    for( int ix = 1; ix < NX-1; ix++ )
    {
        A[(NY-1)][ix] = A[1][ix];
    }
}
```

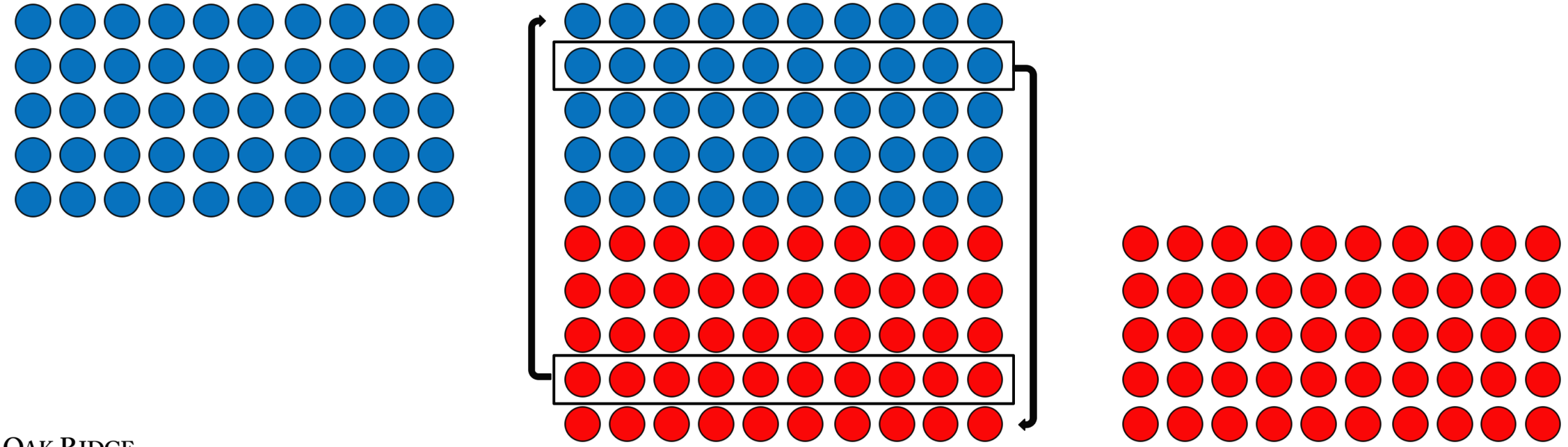
Side Boundaries

Only the threads with (0 == (iy_start-1)) and ((NY-1) == (iy_end)) perform the boundary updates

Thread 0's copy of its rows of A (on GPU 0)

CPU copy of A

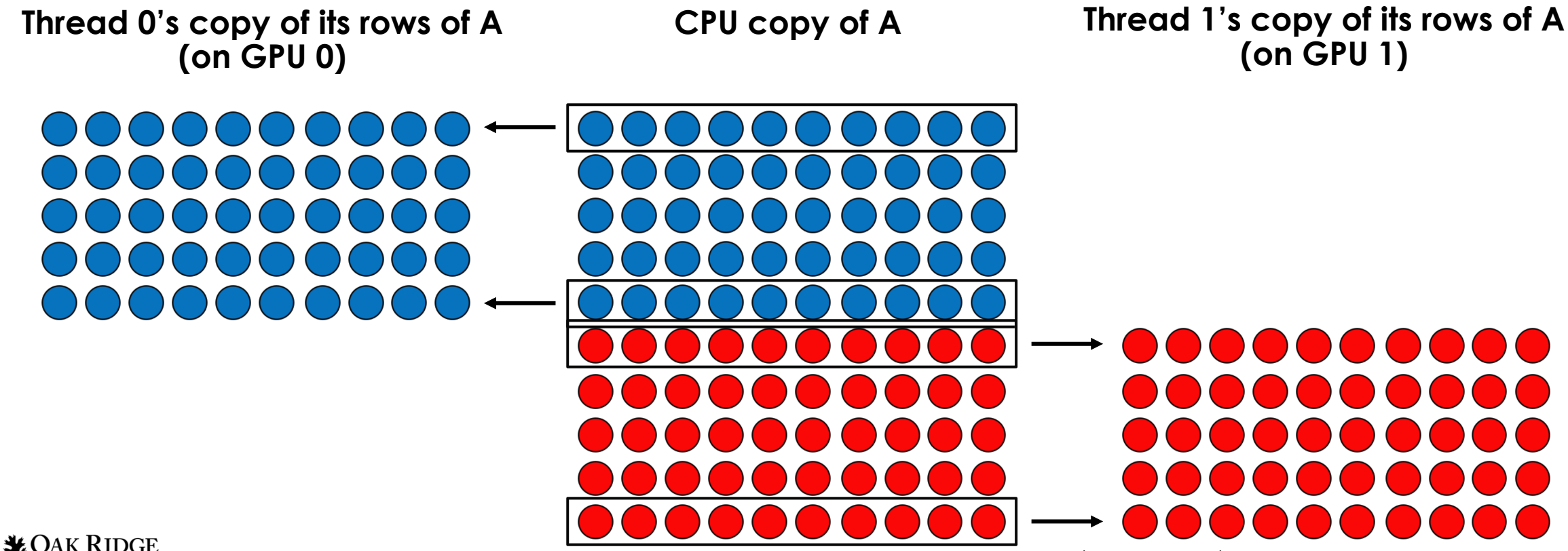
Thread 1's copy of its rows of A (on GPU 1)



Differences from Single GPU Version

```
#pragma acc update device(A[(iy_start-1):1][0:NX], A[iy_end:1][0:NX])
```

Each thread updates its "top" row and "bottom" row from the new values of the CPU copy of A



Runtime of Single GPU Version with Data Directives

Compile the code

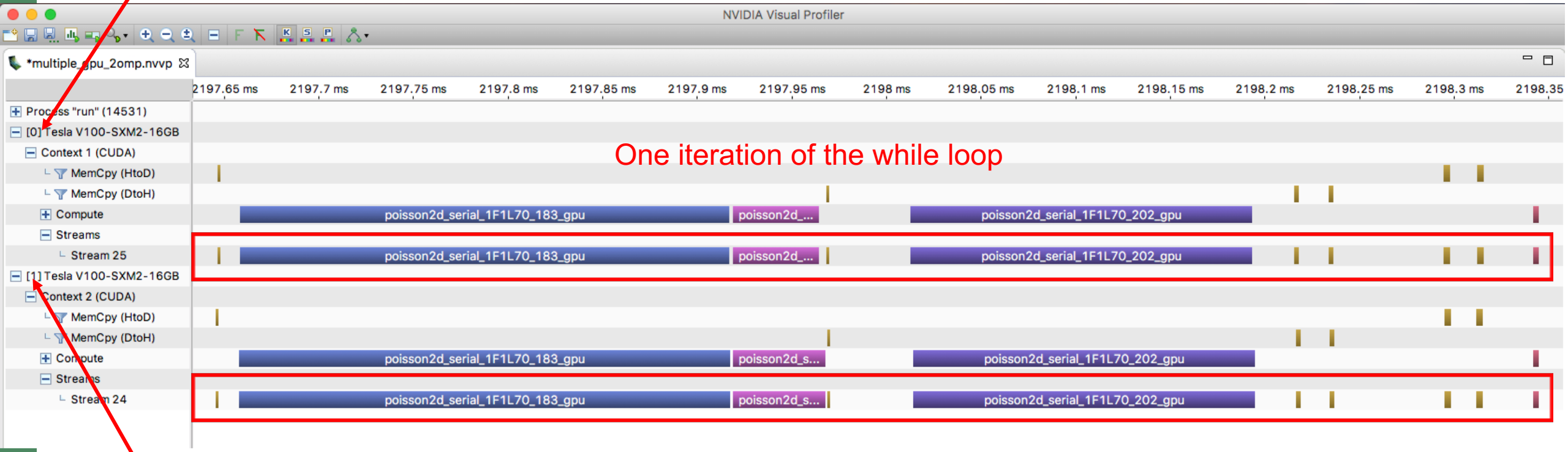
```
$ make
pgcc -acc -Minfo=acc -ta=tesla:cc70 -mp -fast -c poisson2d.c
poisson2d_serial: ...
main:
    103, Generating implicit copyout(A[:][:],A_ref[:][:])
    104, Loop is parallelizable
    106, Loop is parallelizable
         Accelerator kernel generated
         Generating Tesla code
        104, #pragma acc loop gang, vector(4) /* blockIdx.y threadIdx.y */
        106, #pragma acc loop gang, vector(32) /* blockIdx.x threadIdx.x */
    167, Generating copyin(rhs[iy_start:iy_end-iy_start][:])
         Generating create(Anew[iy_start:iy_end-iy_start][:])
         Generating copy(A[iy_start-1:iy_end-iy_start+2][:])
    181, Loop is parallelizable
    183, Loop is parallelizable
         Accelerator kernel generated
         Generating Tesla code
        181, #pragma acc loop gang, vector(4) /* blockIdx.y threadIdx.y */
        183, #pragma acc loop gang, vector(32) /* blockIdx.x threadIdx.x */
        187, Generating implicit reduction(max:error)
    200, Loop is parallelizable
    202, Loop is parallelizable
         Accelerator kernel generated
         Generating Tesla code
        200, #pragma acc loop gang, vector(4) /* blockIdx.y threadIdx.y */
        202, #pragma acc loop gang, vector(32) /* blockIdx.x threadIdx.x */
    211, Generating update self(A[iy_start][:],A[iy_end-1][:])
    230, Generating update device(A[iy_start-1][:],A[iy_end][:])
    231, Loop is parallelizable
         Accelerator kernel generated
         Generating Tesla code
        231, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
pgcc -acc -Minfo=acc -ta=tesla:cc70 -mp -fast poisson2d.o -o run
```

Run the code (on 2 GPUs)

```
$ bsub submit2.lsf

$ less output_2omp
Single-GPU Execution...
    0, 0.250000
  100, 0.249940
  200, 0.249880
  300, 0.249821
  400, 0.249761
  500, 0.249702
  600, 0.249642
  700, 0.249583
  800, 0.249524
  900, 0.249464
Parallel Execution...
    0, 0.250000
  100, 0.249940
  200, 0.249880
  300, 0.249821
  400, 0.249761
  500, 0.249702
  600, 0.249642
  700, 0.249583
  800, 0.249524
  900, 0.249464
Elapsed Time (s) - Serial:     1.0990,
                   Parallel:   0.6692,
                   Speedup:    1.6424
```

Using NVIDIA's Visual Profiler, we see…

OpenMP Thread 0 (GPU 0)



One iteration of the while loop

OpenMP Thread 1 (GPU 1)

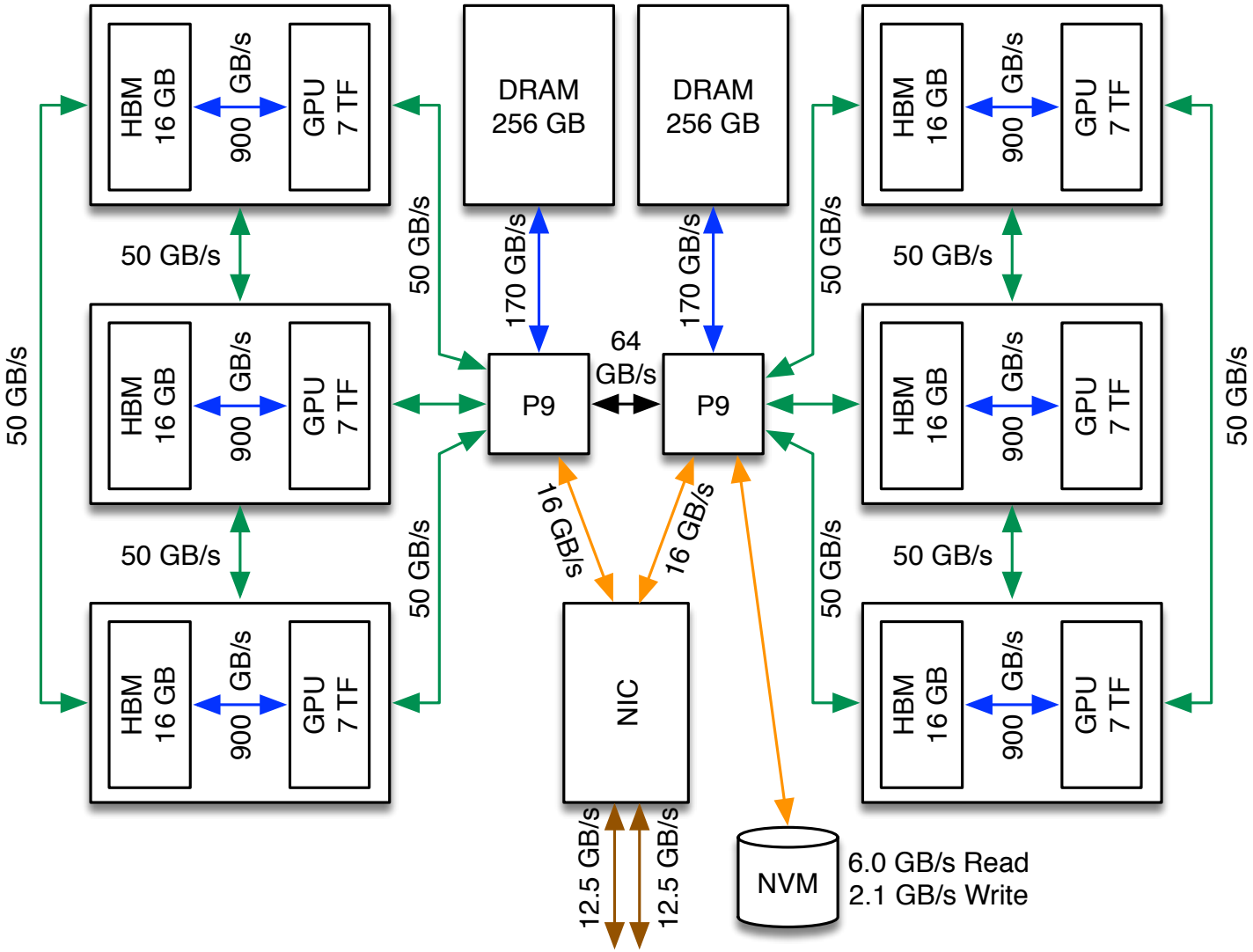
OAK RIDGE National Laboratory

2019_SIAM_CSE/jacobi/4_multiple_gpu_openmp

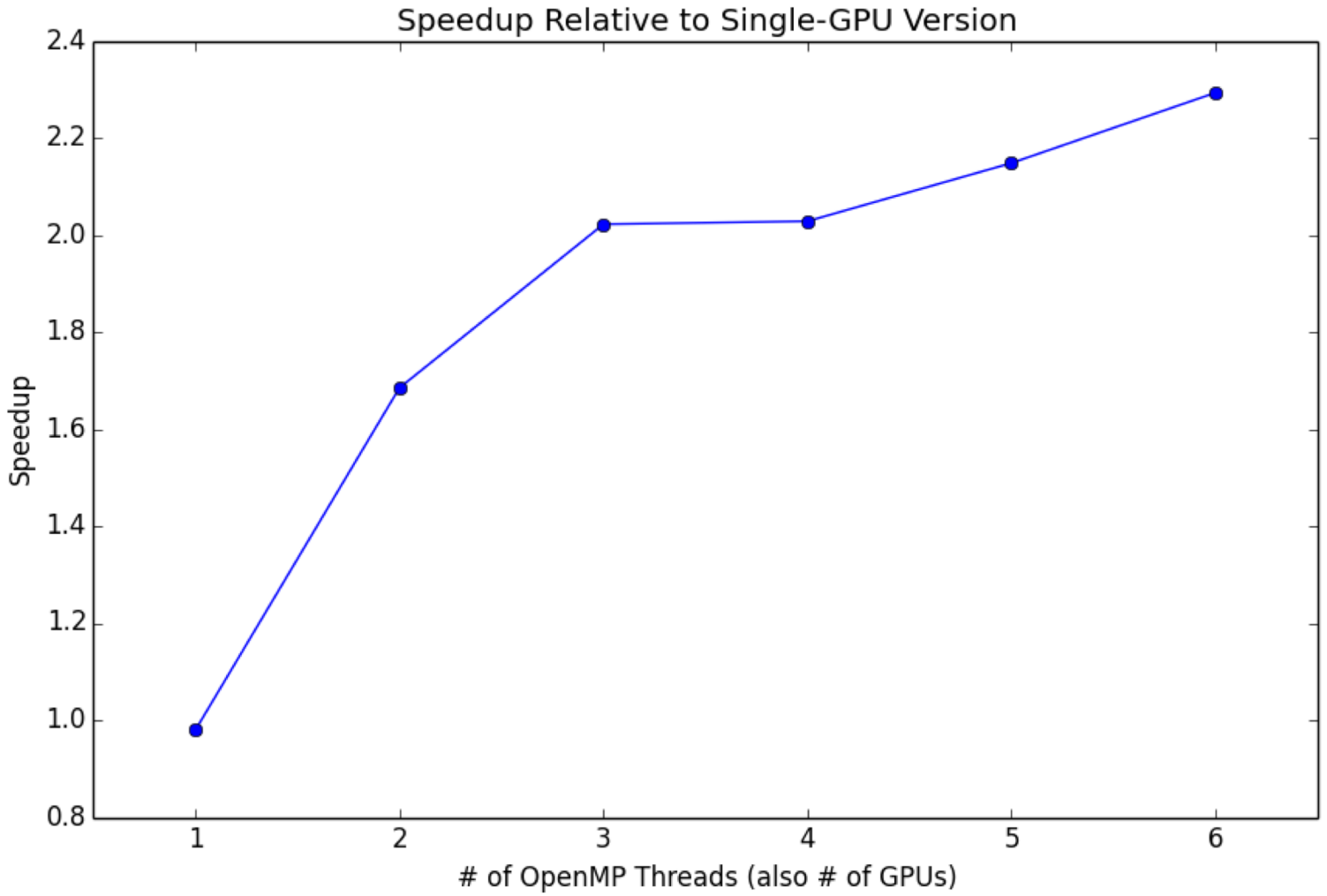
Plot Results of Speedup Versus # of GPUs

Navigate to Google Sheet to enter timing data: https://goo.gl/G2fNeB

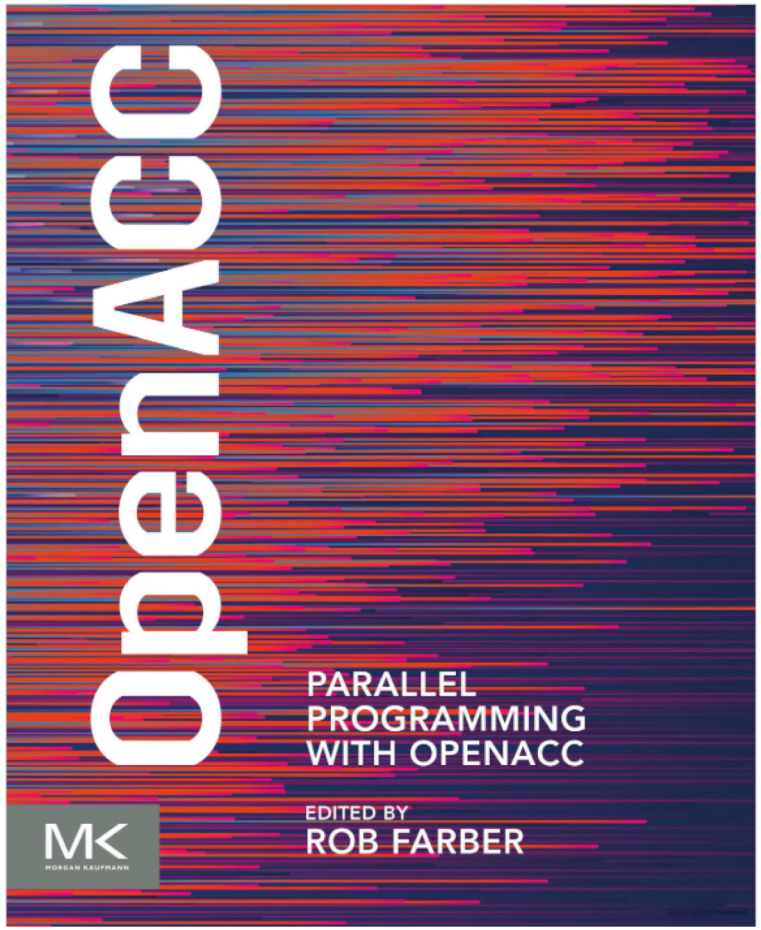
Summit / Ascent Node Overview

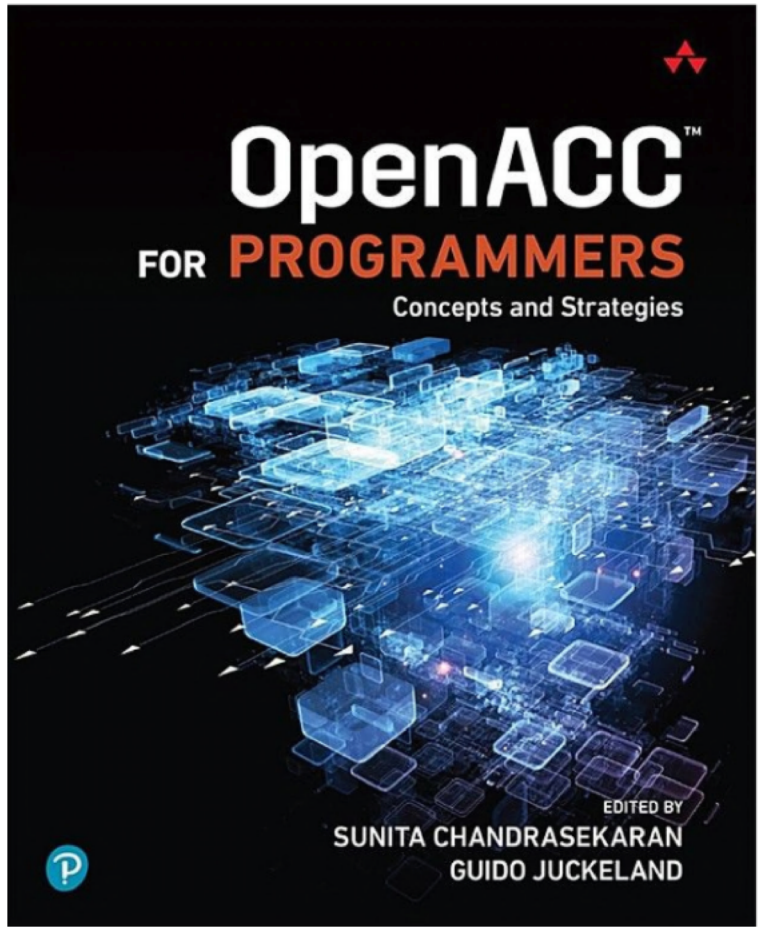


Plot Results of Speedup Versus # of GPUs



Acknowledgements





Thank You.